Electronic Supplementary Information (ESI) for

Interpretation of Tolman Electronic Parameters in the Light of Natural Orbitals for Chemical Valence

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#1 Methods

All calculations were carried out at the density functional (DFT) level of theory with the ADF2014.2 program package.[1] The hybrid functional PBE0[2] was employed for geometry optimization. The PBE0 exchange correlation functional is based on the generalized gradient corrected exchange correlation functional by Perdew-Burke-Ernzerhof (PBE) with a fixed amount of 25% of Hartree-Fock exchange energy. Restricted formalism was applied for all closed shell systems (complexes and fragments). For geometry optimization and fragment analysis C, H, N, O and Cl atoms were described through TZ2P basis sets (triple-ζ STO plus two polarization function); the QZ4P set of basis (quadruple-ζ STO plus four polarization function) was used for Br and Ni atoms. The no-frozen-core approximation (all-electron) and no symmetry constrains were used in all calculations. Complexes geometries were optimized simulating solvent effects (CH_2Cl_2) employing the conductor-like continuum solvent model (COSMO)[3]as implemented in the ADF suite. Frequency calculations were performed for all optimized structures to establish the nature of the stationary points. Plots of calculated *vs.* experimental A_1 ν(CO) are reported in the Supplementary (Figure S1). Analysis of data were performed with Origin 8.0 (OriginLab, Northampton, MA) and Maxima, a Computer Algebra System. Version 5.38.1 (2016) (http://maxima.sourceforge.net).

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(b) C. Fonseca Guerra, J. G. Snijders, G. te Velde and E. J. Baerends, *Theor. Chem. Acc.* 1998, **99**, 391-403;
(c) ADF2014, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com. Full list of authors: E.J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, J.W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, H. van Schoot, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev.

[2] J. P. Perdew, M. Ernzerhof, K. Burke *J. Chem. Phys.* **105**, 9982-9985 (1996).

[3] A. Klamt, G. Schüürmann *J. Chem. Soc. Perkin Trans.* **2**, 799-805 (1993).

#2 Results of geometry optimization

1 $P(C_6F_5)_3$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	F	0.000059	0.000048	-0.000010
2	F	-0.000052	0.000002	0.000063
3	P	0.000129	-0.000213	0.000192
4	F	0.000029	0.000004	0.000062
5	F	-0.000038	-0.000002	0.000068
6	C	0.000280	0.000129	-0.000287
7	O	-0.000226	0.000044	-0.000015
8	C	-0.000016	0.000048	0.000379
9	F	0.000020	0.000042	-0.000002
10	F	-0.000038	0.000024	0.000110
11	C	0.000349	-0.000135	0.000000
12	F	0.000071	-0.000015	-0.000036
13	F	0.000039	-0.000050	-0.000018
14	Ni	-0.000330	0.000139	-0.000030
15	O	-0.000162	-0.000071	0.000132
16	O	0.000019	-0.000041	-0.000203
17	F	-0.000095	0.000034	-0.000013
18	C	-0.000127	-0.000018	0.000008
19	C	-0.000133	0.000069	0.000007
20	C	0.000019	0.000116	0.000043
21	C	-0.000017	-0.000134	-0.000023
22	C	-0.000117	-0.000047	0.000048
23	C	0.000192	-0.000063	-0.000071
24	C	0.000239	0.000047	-0.000311
25	C	-0.000080	-0.000001	0.000223
26	C	0.000039	-0.000049	-0.000146
27	C	0.000122	0.000024	-0.000053
28	C	-0.000091	-0.000035	-0.000040
29	C	-0.000008	-0.000009	-0.000036
30	F	-0.000025	0.000018	-0.000069
31	C	-0.000026	0.000169	0.000124
32	C	0.000054	0.000109	-0.000044
33	C	0.000006	0.000019	-0.000104
34	C	-0.000017	-0.000035	0.000144
35	C	0.000063	0.000198	-0.000027
36	C	-0.000136	-0.000265	-0.000059
37	F	-0.000023	-0.000027	0.000025
38	F	-0.000015	-0.000058	0.000037
39	F	-0.000010	-0.000031	-0.000039
40	F	0.000005	-0.000038	-0.000013
41	F	0.000045	0.000052	-0.000017

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2 $P(OMe)_3$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	-0.000383	0.002182	0.000846
2	O	0.006747	-0.000273	-0.001911
3	P	-0.005110	0.004071	-0.000724
4	O	0.000162	-0.000370	-0.000257
5	O	0.000485	-0.001323	-0.004136
6	C	-0.005869	0.001496	0.001958
7	C	-0.001337	0.000421	0.000309
8	C	0.000267	0.000695	0.003374
9	H	-0.000396	-0.000653	-0.000547
10	H	-0.000087	0.000273	0.000153
11	H	0.002019	-0.000396	0.000436
12	O	-0.001348	0.000443	0.000967
13	C	-0.000581	-0.000352	-0.000103
14	H	-0.000441	-0.000235	0.000136
15	H	0.000175	-0.000422	-0.000691
16	O	0.001387	-0.000309	-0.000027
17	C	0.003543	-0.003547	-0.002629
18	H	0.000780	0.000480	0.001055
19	H	-0.000231	-0.000593	-0.001563
20	O	-0.000289	-0.001479	-0.000353
21	C	0.000054	-0.000700	0.002312
22	H	0.000145	0.000175	-0.000938
23	H	0.000309	0.000416	0.002335

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3 $P(OMe)Ph_2$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	-0.000298	0.000022	0.000229
2	O	-0.000036	-0.000211	-0.000089
3	P	-0.000237	-0.000048	0.000211
4	O	-0.000207	0.000011	0.000142
5	O	-0.000314	-0.000273	0.000049
6	C	0.000114	0.000115	0.000044
7	C	0.000272	-0.000012	-0.000112
8	C	0.000393	0.000316	-0.000149
9	C	-0.000056	-0.000019	-0.000195
10	H	0.000016	0.000123	0.000062
11	H	-0.000126	0.000135	0.000165
12	H	0.000013	-0.000011	-0.000018
13	H	-0.000047	0.000161	0.000185
14	H	-0.000006	0.000024	-0.000023
15	O	0.000778	-0.000048	-0.000245
16	C	-0.000046	-0.000083	-0.000059
17	C	0.000018	-0.000008	0.000088
18	C	0.000018	-0.000052	-0.000062
19	C	-0.000031	0.000025	-0.000054
20	C	-0.000001	0.000001	-0.000020
21	C	-0.000017	0.000019	0.000023
22	H	-0.000031	0.000002	-0.000020
23	H	-0.000039	-0.000003	0.000000
24	H	-0.000032	-0.000015	0.000013
25	H	-0.000008	-0.000040	-0.000006
26	C	0.000016	0.000002	-0.000186
27	C	0.000060	-0.000044	0.000093
28	C	0.000015	0.000063	-0.000123
29	C	-0.000072	0.000011	-0.000005
30	C	-0.000041	0.000007	-0.000023
31	C	0.000001	-0.000086	0.000127
32	H	-0.000055	-0.000007	-0.000028
33	H	-0.000022	-0.000043	0.000000
34	H	0.000005	-0.000037	0.000003
35	H	0.000002	0.000003	-0.000020

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4 $P(OPh)_3$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	-0.000700	0.000128	-0.000273
2	O	-0.000152	0.000079	0.000032
3	P	-0.000148	-0.000015	-0.000224
4	O	0.000230	0.000383	-0.000234
5	O	-0.000328	-0.000023	-0.000194
6	C	0.000286	0.000013	0.000008
7	C	-0.000204	-0.000515	0.000130
8	C	0.000509	0.000055	0.000340
9	H	-0.000193	-0.000119	0.000032
10	H	0.000057	0.000070	0.000041
11	H	-0.000230	0.000154	-0.000029
12	O	-0.000095	0.000405	0.000006
13	O	0.000282	-0.000043	-0.000169
14	O	-0.000151	0.000068	0.000563
15	C	0.000343	-0.000245	-0.000006

16	C	0.000149	0.000149	0.000061
17	C	0.000213	-0.000239	-0.000167
18	C	0.000060	-0.000008	0.000034
19	C	-0.000173	-0.000021	-0.000136
20	C	-0.000021	0.000145	0.000012
21	H	0.000269	-0.000100	0.000000
22	H	0.000325	-0.000173	-0.000053
23	H	0.000111	-0.000038	-0.000056
24	H	-0.000134	0.000119	-0.000065
25	C	-0.000069	0.000009	0.000005
26	C	0.000032	0.000164	0.000148
27	C	-0.000163	-0.000234	-0.000150
28	C	-0.000089	0.000094	-0.000010
29	C	-0.000116	0.000005	-0.000021
30	C	-0.000046	-0.000168	0.000054
31	H	-0.000059	0.000049	-0.000049
32	H	-0.000150	0.000007	0.000047
33	H	-0.000131	-0.000076	0.000068
34	H	-0.000096	-0.000119	-0.000025
35	C	0.000178	-0.000059	-0.000305
36	C	-0.000038	0.000056	-0.000104
37	C	0.000038	-0.000041	0.000054
38	C	0.000168	0.000052	0.000267
39	C	-0.000083	0.000137	-0.000322
40	C	0.000138	-0.000145	0.000308
41	H	-0.000015	-0.000031	0.000044
42	H	0.000059	-0.000021	0.000041
43	H	0.000090	0.000034	0.000133
44	H	0.000044	0.000058	0.000165

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5 **$P(Ph)Cl_2$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000504	0.000065	-0.000044
2	O	0.000036	0.000045	-0.000037
3	P	-0.000320	0.000032	0.000186
4	O	0.000060	0.000001	0.000030
5	O	-0.000087	-0.000092	0.000185
6	C	-0.000165	0.000047	0.000153
7	C	-0.000250	-0.000042	0.000079
8	C	-0.000014	-0.000013	-0.000336
9	Cl	0.000190	0.000114	-0.000205
10	Cl	0.000035	-0.000122	-0.000019
11	H	0.000025	-0.000013	0.000037
12	C	-0.000021	-0.000113	0.000037
13	C	-0.000002	-0.000004	-0.000007
14	C	0.000003	0.000000	-0.000009
15	C	0.000015	-0.000038	0.000015
16	C	0.000025	0.000092	0.000047
17	C	-0.000030	0.000018	-0.000096
18	H	0.000004	0.000019	-0.000013
19	H	0.000015	0.000032	0.000000
20	H	-0.000005	-0.000007	0.000004
21	H	-0.000018	-0.000021	-0.000006

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6 **PCl_3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000244	-0.000163	0.000114
2	O	-0.000166	0.000228	0.000112
3	P	-0.000012	-0.000035	0.000015
4	O	0.000023	-0.000045	0.000115
5	O	0.000201	0.000234	0.000215
6	C	-0.000095	-0.000152	-0.000028
7	C	0.000215	0.000166	-0.000190
8	C	-0.000440	-0.000317	-0.000277
9	Cl	0.000108	0.000056	-0.000041
10	Cl	-0.000057	0.000051	0.000023
11	Cl	-0.000020	-0.000023	-0.000057

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7 **$P(Ph)_2Cl$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	-0.000274	-0.000154	-0.000132
2	O	-0.000006	-0.000117	0.000160
3	P	0.000150	-0.000062	0.000127
4	O	-0.000200	0.000179	0.000059
5	O	-0.000109	-0.000095	0.000174
6	C	0.000046	0.000292	-0.000195
7	C	0.000248	-0.000177	0.000009
8	C	0.000248	0.000172	-0.000223
9	Cl	-0.000030	-0.000011	0.000015
10	H	0.000003	-0.000012	0.000001
11	H	0.000014	0.000004	0.000036
12	C	-0.000066	-0.000216	-0.000035
13	C	-0.000077	0.000076	-0.000024
14	C	0.000034	0.000100	0.000022
15	C	0.000057	-0.000092	0.000042
16	C	-0.000007	0.000049	-0.000106
17	C	0.000052	0.000078	0.000006
18	H	0.000037	0.000002	0.000003
19	H	-0.000012	-0.000026	-0.000011
20	H	-0.000013	-0.000013	0.000008
21	H	-0.000041	-0.000006	0.000016
22	C	-0.000115	-0.000037	0.000146
23	C	0.000012	0.000095	-0.000110
24	C	-0.000067	-0.000044	0.000077
25	C	0.000073	0.000057	-0.000032
26	C	-0.000045	-0.000045	-0.000082
27	C	0.000054	0.000044	-0.000020
28	H	0.000005	-0.000031	0.000018
29	H	0.000015	0.000003	0.000008
30	H	0.000000	-0.000002	0.000011
31	H	0.000016	-0.000009	0.000034

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8 **PEt_3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000061	0.000131	-0.000025
2	H	0.000111	0.000024	0.000050
3	P	0.000538	-0.000477	0.000263
4	H	0.000003	-0.000025	-0.000202
5	H	0.000031	0.000050	-0.000013
6	H	0.000028	0.000039	-0.000196
7	H	-0.000143	0.000049	0.000111
8	H	0.000095	-0.000013	0.000122
9	C	0.000845	-0.000170	-0.000185
10	C	-0.000136	0.000254	0.000612
11	C	-0.000806	-0.000403	0.000237
12	H	-0.000081	0.000271	0.000164
13	H	-0.000044	-0.000056	-0.000097
14	Ni	-0.000228	0.000190	-0.000245
15	O	-0.000074	0.000055	0.000130
16	O	0.000212	0.000062	-0.000070
17	O	0.000438	0.000426	0.000514
18	C	0.000087	-0.000002	-0.000162
19	C	-0.000328	-0.000135	0.000119
20	C	-0.000321	-0.000334	-0.000397
21	C	0.000155	0.000203	0.000069
22	H	-0.000072	0.000029	-0.000050
23	H	0.000181	0.000121	-0.000227

24	C	0.000153	-0.000026	-0.000315
25	H	-0.000396	-0.000230	-0.000173
26	H	0.000098	0.000084	0.000091
27	C	-0.000273	-0.000094	0.000069
28	H	0.000047	-0.000057	0.000006
29	H	-0.000058	0.000033	-0.000202

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9 **PF_3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000367	-0.000788	0.000676
2	O	-0.000499	-0.000040	0.000356
3	P	-0.000255	0.000443	-0.000293
4	O	0.000152	-0.000175	0.000129
5	O	-0.000091	0.000052	0.000308
6	C	0.000502	0.000121	-0.000425
7	C	-0.000201	0.000208	-0.000165
8	C	0.000098	0.000043	-0.000443
9	F	0.000546	0.000234	-0.000298
10	F	-0.000282	0.000337	0.000452
11	F	-0.000335	-0.000435	-0.000295

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10 **$PH_2(Ph)$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000621	-0.000583	0.000859
2	O	0.000345	-0.000410	-0.000232
3	P	-0.000475	-0.000107	-0.000472
4	O	-0.000384	-0.000434	0.000511
5	O	-0.000137	-0.000280	-0.000186
6	C	-0.000346	0.000447	0.000195
7	C	0.000352	0.000390	-0.000540
8	C	-0.000097	0.000219	-0.000011
9	H	0.000437	0.000229	-0.000403
10	H	-0.000278	0.000512	0.000253
11	H	0.000012	0.000006	0.000027
12	C	-0.000099	0.000010	0.000039
13	C	0.000033	-0.000006	-0.000034
14	C	0.000001	-0.000013	0.000015
15	C	0.000009	0.000007	0.000036
16	C	-0.000001	-0.000040	-0.000068
17	C	0.000053	0.000038	-0.000019
18	H	-0.000019	0.000003	0.000005
19	H	-0.000003	0.000006	0.000010
20	H	-0.000001	-0.000005	0.000006
21	H	-0.000023	0.000011	0.000009

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11 **$PH(Ph)_2$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	-0.000242	-0.000071	0.000101
2	O	0.000056	-0.000146	-0.000045
3	P	0.000047	-0.000064	-0.000180
4	O	-0.000157	-0.000129	0.000136
5	O	-0.000021	0.000046	0.000086
6	C	0.000061	0.000166	0.000024
7	C	0.000140	0.000169	-0.000180
8	C	0.000149	-0.000050	-0.000128
9	H	-0.000022	-0.000020	-0.000008
10	H	-0.000029	0.000030	0.000003
11	H	0.000017	-0.000007	-0.000039
12	C	0.000016	0.000046	0.000010
13	C	0.000024	0.000002	0.000019
14	C	-0.000026	0.000000	-0.000030
15	C	-0.000018	-0.000013	0.000054
16	C	0.000006	-0.000007	-0.000076
17	C	0.000045	-0.000002	0.000098
18	H	0.000002	-0.000018	-0.000011
19	H	0.000013	-0.000008	0.000003
20	H	0.000004	-0.000002	-0.000005
21	H	-0.000012	0.000001	0.000022
22	C	-0.000242	0.000023	0.000208
23	C	0.000071	0.000117	0.000094
24	C	0.000069	-0.000059	-0.000171
25	C	-0.000137	-0.000076	0.000036
26	C	0.000027	0.000186	0.000072
27	C	0.000142	-0.000121	-0.000122
28	H	-0.000002	0.000024	-0.000015
29	H	0.000032	0.000005	0.000021
30	H	0.000006	-0.000012	0.000028
31	H	-0.000021	-0.000012	-0.000004

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12 **$PMe_2(CF_3)$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000008	-0.000014	-0.000006
2	H	-0.000007	-0.000011	-0.000009
3	P	-0.000482	0.000371	-0.000521
4	H	-0.000019	0.000009	-0.000005
5	H	-0.000028	-0.000021	-0.000010
6	F	0.000212	0.000057	-0.000296
7	F	0.000060	-0.000182	0.000075
8	F	-0.000277	0.000114	0.000243
9	C	0.000049	0.000048	0.000075
10	C	0.000076	0.000007	0.000069
11	C	0.000097	0.000081	0.000028
12	H	-0.000007	-0.000026	-0.000018
13	H	-0.000008	0.000004	-0.000015
14	Ni	0.000417	-0.000515	0.000504
15	O	0.000326	-0.000456	-0.000427
16	O	0.000154	0.000072	-0.000199
17	O	-0.000466	-0.000377	-0.000349
18	C	-0.000377	0.000465	0.000432
19	C	-0.000125	-0.000037	0.000191
20	C	0.000413	0.000412	0.000239

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13 **PMe_2Ph**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000144	0.000093	0.000052
2	H	0.000038	-0.000087	-0.000043
3	P	0.000194	0.000413	-0.000120
4	H	0.000048	-0.000012	-0.000053
5	H	0.000062	-0.000123	0.000029
6	C	0.000204	0.000279	-0.000055
7	O	-0.000085	0.000023	-0.000183
8	C	0.000432	-0.000325	-0.000109
9	C	-0.000302	-0.000454	-0.000055
10	C	-0.000258	0.000347	0.000082
11	C	0.000237	0.000084	0.000327
12	H	0.000002	0.000090	0.000149
13	H	0.000135	0.000052	-0.000018
14	Ni	-0.000322	-0.000126	-0.000171
15	O	-0.000197	-0.000166	0.000138
16	O	-0.000256	0.000080	0.000068
17	H	-0.000019	0.000063	-0.000001

18	C	-0.000016	-0.000168	-0.000089
19	C	0.000003	0.000115	0.000072
20	C	-0.000114	-0.000041	-0.000056
21	C	0.000097	0.000087	-0.000063
22	C	0.000022	-0.000032	0.000109
23	C	-0.000055	-0.000110	-0.000018
24	H	0.000047	-0.000069	0.000026
25	H	-0.000001	-0.000035	0.000005
26	H	-0.000021	0.000005	0.000008
27	H	-0.000018	0.000019	-0.000030

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14 **PMe_3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000119	0.000029	0.000048
2	H	0.000042	-0.000029	-0.000140
3	P	0.000185	0.000078	-0.000105
4	H	-0.000001	0.000040	-0.000079
5	H	-0.000038	0.000077	0.000067
6	H	0.000064	0.000016	-0.000018
7	H	0.000035	-0.000067	0.000040
8	H	-0.000011	0.000106	-0.000001
9	C	-0.000015	0.000020	-0.000003
10	C	-0.000004	-0.000090	0.000050
11	C	-0.000013	-0.000060	0.000033
12	H	0.000033	-0.000059	0.000072
13	H	-0.000037	-0.000041	-0.000026
14	Ni	-0.000331	0.000138	0.000308
15	O	-0.000096	0.000117	0.000092
16	O	-0.000224	0.000094	0.000071
17	O	-0.000129	0.000020	-0.000026
18	C	0.000252	-0.000186	-0.000311
19	C	0.000342	-0.000070	-0.000018
20	C	0.000064	-0.000134	-0.000054

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15 **$PMePh_2$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000005	-0.000015	0.000023
2	H	0.000015	0.000035	0.000003
3	P	-0.000055	0.000121	-0.000016
4	H	0.000051	-0.000009	0.000011
5	H	0.000021	0.000004	0.000016
6	C	-0.000179	-0.000113	0.000024
7	O	-0.000041	-0.000017	-0.000042
8	C	-0.000207	0.000059	0.000148
9	H	-0.000008	-0.000032	0.000028
10	C	-0.000142	-0.000112	-0.000064
11	C	0.000135	0.000054	0.000008
12	H	0.000027	-0.000025	0.000027
13	H	-0.000012	-0.000008	-0.000007
14	Ni	0.000266	-0.000240	0.000137
15	O	0.000114	0.000120	0.000009
16	O	0.000087	-0.000043	-0.000088
17	H	-0.000036	-0.000022	0.000060
18	C	-0.000347	0.000193	0.000114
19	C	0.000156	0.000097	-0.000106
20	C	0.000005	-0.000099	0.000001
21	C	0.000026	0.000036	0.000012
22	C	-0.000074	-0.000007	-0.000106
23	C	0.000234	0.000003	-0.000095
24	C	0.000169	0.000088	-0.000368
25	C	-0.000108	-0.000074	0.000099
26	C	-0.000029	0.000093	-0.000022
27	C	-0.000003	-0.000074	0.000050
28	C	0.000045	0.000057	-0.000065
29	C	-0.000154	-0.000032	0.000213
30	H	0.000034	-0.000003	0.000011
31	H	0.000008	-0.000008	-0.000009
32	H	0.000009	-0.000006	-0.000003
33	H	-0.000021	-0.000013	0.000009
34	H	0.000019	-0.000008	-0.000012

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16 **$P(NMe_2)_3$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000142	0.000326	0.000205
2	O	-0.000306	-0.000026	0.000186
3	P	0.000679	-0.000190	-0.000474
4	O	-0.000167	-0.000347	-0.000069
5	O	0.000016	0.000188	-0.000040
6	C	0.000264	-0.000077	-0.000556
7	C	0.000171	0.000367	0.000057
8	C	-0.000076	-0.000354	0.000343
9	H	-0.000042	0.000090	0.000119
10	H	0.000000	0.000042	-0.000048
11	H	-0.000026	-0.000006	0.000024
12	N	0.000032	-0.000392	-0.000170
13	C	-0.000077	0.000064	0.000494
14	H	0.000129	0.000209	-0.000086
15	H	0.000202	-0.000189	-0.000245
16	N	-0.000027	0.000363	-0.000162
17	C	-0.000528	0.000035	0.000464
18	H	-0.000045	0.000035	0.000006
19	H	-0.000011	-0.000043	0.000148
20	N	-0.000002	-0.000004	0.000184
21	C	-0.000151	-0.000191	-0.000077
22	H	0.000004	0.000016	-0.000015
23	H	-0.000001	-0.000003	0.000007
24	C	-0.000043	-0.000232	-0.000142
25	H	0.000051	0.000048	0.000064
26	H	0.000067	-0.000021	0.000083
27	H	-0.000020	0.000035	0.000005
28	C	-0.000214	-0.000190	-0.000416
29	H	0.000142	0.000351	0.000193
30	H	0.000180	0.000086	0.000036
31	H	0.000036	-0.000078	0.000026
32	C	-0.000570	0.000521	-0.000633
33	H	0.000343	-0.000382	0.000349
34	H	-0.000165	-0.000029	0.000141
35	H	0.000014	-0.000024	0.000000

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17 **PPh_3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000012	-0.000007	0.000023
2	H	-0.000010	-0.000012	-0.000003
3	P	0.000236	-0.000421	0.000406
4	H	0.000031	-0.000037	-0.000014
5	H	0.000007	-0.000001	0.000016
6	C	0.000014	-0.000209	-0.000150
7	O	0.000050	0.000034	0.000030
8	C	-0.000082	-0.000081	0.000136
9	H	-0.000010	0.000005	0.000021
10	H	0.000091	-0.000030	-0.000027
11	C	0.000164	0.000124	-0.000006
12	H	0.000009	-0.000016	-0.000037
13	H	0.000003	-0.000013	0.000029
14	Ni	-0.000516	0.000440	-0.000393

15	O	0.000020	0.000080	0.000076
16	O	0.000000	-0.000011	-0.000083
17	H	0.000034	0.000037	0.000009
18	C	0.000182	0.000108	0.000185
19	C	-0.000110	-0.000032	-0.000105
20	C	0.000016	-0.000003	0.000010
21	C	-0.000025	-0.000002	-0.000087
22	C	-0.000004	0.000015	0.000017
23	C	-0.000036	-0.000049	-0.000021
24	C	0.000044	0.000022	-0.000211
25	C	-0.000053	-0.000033	0.000125
26	C	-0.000018	0.000003	-0.000107
27	C	0.000019	-0.000035	0.000033
28	C	0.000014	0.000131	-0.000004
29	C	-0.000135	0.000030	0.000043
30	H	-0.000005	-0.000026	0.000000
31	C	-0.000008	0.000102	0.000100
32	C	-0.000007	-0.000096	-0.000064
33	C	-0.000065	0.000036	0.000061
34	C	0.000075	-0.000015	-0.000050
35	C	-0.000125	0.000012	0.000034
36	C	0.000054	-0.000032	0.000032
37	H	0.000036	-0.000048	0.000005
38	H	0.000018	0.000014	0.000035
39	H	0.000005	0.000009	-0.000036
40	H	0.000035	-0.000019	-0.000014
41	H	0.000040	0.000025	-0.000013

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18 **PEt_2Ph**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000022	0.000005	-0.000049
2	H	0.000099	0.000302	0.000209
3	P	0.000343	0.000489	0.000596
4	H	0.000491	-0.000057	-0.000009
5	H	-0.000039	-0.000080	-0.000051
6	C	0.000243	-0.000498	-0.000392
7	O	-0.000224	-0.000196	-0.000097
8	C	-0.000261	0.000100	0.000243
9	C	-0.000543	0.000187	0.000269
10	C	-0.000700	-0.000875	-0.000888
11	C	0.000330	0.000236	0.000083
12	H	-0.000062	-0.000214	-0.000031
13	H	0.000090	0.000058	-0.000021
14	Ni	-0.000061	0.000264	-0.000253
15	O	-0.000097	0.000283	0.000333
16	O	0.000039	0.000010	-0.000219
17	H	-0.000087	0.000023	0.000068
18	C	0.000193	-0.000242	0.000264
19	C	-0.000180	0.000260	-0.000017
20	C	0.000133	-0.000253	-0.000012
21	C	0.000019	0.000118	0.000013
22	C	-0.000080	-0.000020	-0.000090
23	C	0.000131	0.000221	-0.000289
24	H	-0.000018	-0.000240	0.000042
25	H	-0.000061	0.000079	0.000023
26	H	-0.000044	-0.000002	0.000057
27	H	0.000013	-0.000034	-0.000037
28	C	0.000059	0.000001	-0.000087
29	H	0.000053	-0.000168	0.000177
30	H	0.000027	0.000094	0.000008
31	C	-0.000173	-0.000060	0.000026
32	H	0.000362	0.000111	0.000113
33	H	0.000025	0.000096	0.000020

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19 **$PEtPh_2$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000005	-0.000005	-0.000021
2	H	0.000004	-0.000014	-0.000013
3	P	-0.000155	0.000256	0.000022
4	H	0.000026	0.000014	-0.000005
5	H	-0.000002	-0.000008	0.000004
6	C	-0.000021	0.000030	0.000041
7	O	0.000013	0.000043	0.000056
8	C	0.000028	0.000017	-0.000065
9	H	-0.000011	-0.000001	0.000015
10	C	-0.000042	-0.000188	-0.000125
11	C	-0.000041	-0.000085	-0.000124
12	H	0.000012	-0.000029	-0.000004
13	H	0.000009	-0.000007	-0.000033
14	Ni	0.000173	0.000039	0.000260
15	O	0.000028	-0.000106	-0.000084
16	O	-0.000070	-0.000054	0.000058
17	H	0.000011	-0.000006	0.000024
18	C	0.000033	0.000033	-0.000041
19	C	0.000015	0.000032	-0.000013
20	C	-0.000032	-0.000073	0.000085
21	C	-0.000007	0.000079	0.000047
22	C	0.000027	-0.000008	-0.000019
23	C	0.000002	0.000029	-0.000096
24	C	-0.000117	-0.000044	-0.000035
25	C	0.000073	0.000027	-0.000015
26	C	-0.000020	0.000087	0.000074
27	C	0.000030	-0.000092	-0.000084
28	C	-0.000038	-0.000026	0.000028
29	C	0.000028	0.000069	-0.000020
30	H	0.000007	-0.000009	-0.000005
31	H	0.000025	-0.000011	-0.000010
32	H	-0.000009	0.000017	0.000003
33	H	0.000017	0.000015	-0.000011
34	H	-0.000014	-0.000040	0.000029
35	C	-0.000021	0.000018	0.000083
36	H	0.000003	-0.000001	0.000008
37	H	0.000030	0.000001	-0.000013

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20 **$PPh(OEt)_2$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000082	0.000224	-0.000131
2	O	0.000094	0.000140	0.000105
3	P	-0.000122	0.000112	0.000128
4	O	-0.000187	-0.000241	0.000014
5	O	-0.000089	0.000117	0.000164
6	C	-0.000173	-0.000168	-0.000177
7	C	0.000200	0.000155	-0.000027
8	C	0.000020	-0.000105	-0.000035
9	H	-0.000013	0.000001	-0.000031
10	H	0.000009	-0.000013	0.000010
11	H	-0.000007	-0.000018	-0.000023
12	C	-0.000010	0.000052	-0.000085
13	C	0.000008	-0.000058	0.000075
14	C	-0.000006	-0.000001	0.000006
15	C	-0.000002	0.000017	-0.000022
16	C	-0.000030	-0.000035	0.000006
17	C	0.000034	0.000028	0.000045
18	H	0.000007	0.000028	-0.000020
19	H	-0.000004	-0.000003	-0.000015
20	H	-0.000002	0.000010	-0.000001
21	H	0.000010	0.000001	0.000003

22	O	0.000037	-0.000204	0.000148
23	C	0.000003	0.000014	-0.000084
24	H	-0.000016	0.000012	0.000031
25	H	0.000000	-0.000016	0.000009
26	O	0.000164	-0.000066	-0.000131
27	C	-0.000147	-0.000009	0.000035
28	H	0.000028	0.000030	-0.000011
29	H	0.000051	0.000004	0.000008
30	C	0.000107	-0.000016	0.000067
31	H	-0.000015	0.000007	-0.000032
32	H	-0.000033	0.000004	-0.000018
33	C	0.000003	0.000003	-0.000040
34	H	-0.000002	-0.000007	0.000013
35	H	-0.000001	0.000001	0.000012

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21 $PPh_2(C_6F_5)$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	F	0.000065	-0.000003	-0.000009
2	H	0.000006	-0.000015	-0.000001
3	P	-0.000106	0.000166	-0.000121
4	H	-0.000002	-0.000019	0.000003
5	H	0.000007	0.000001	-0.000020
6	C	0.000205	-0.000482	-0.000159
7	O	-0.000378	-0.000215	-0.000198
8	C	-0.000242	-0.000008	0.000093
9	F	0.000031	0.000007	0.000102
10	H	-0.000012	0.000033	0.000035
11	C	0.000395	0.000056	0.000265
12	F	0.000048	-0.000035	0.000070
13	F	0.000037	-0.000006	0.000076
14	Ni	0.000043	-0.000011	0.000181
15	O	-0.000158	0.000519	0.000180
16	O	0.000243	0.000103	-0.000250
17	F	-0.000033	-0.000036	0.000019
18	C	0.000098	-0.000069	0.000383
19	C	0.000077	-0.000025	-0.000301
20	C	-0.000076	-0.000103	-0.000151
21	C	-0.000074	0.000064	0.000150
22	C	0.000083	0.000087	-0.000141
23	C	-0.000121	0.000074	-0.000119
24	C	-0.000046	-0.000009	-0.000086
25	C	0.000026	-0.000036	0.000040
26	C	-0.000036	0.000050	-0.000014
27	C	0.000040	-0.000031	0.000033
28	C	-0.000027	0.000011	0.000006
29	C	-0.000041	0.000030	0.000002
30	H	0.000000	0.000034	0.000031
31	C	-0.000397	-0.000144	-0.000055
32	C	0.000215	0.000103	-0.000005
33	C	0.000017	-0.000071	-0.000064
34	C	-0.000118	-0.000023	0.000069
35	C	-0.000088	0.000073	0.000043
36	C	0.000256	-0.000052	0.000005
37	H	0.000028	-0.000038	-0.000042
38	H	-0.000065	-0.000003	0.000016
39	H	0.000120	0.000005	-0.000034
40	H	-0.000047	-0.000004	0.000009
41	H	0.000029	0.000024	-0.000039

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22 $PPh_2(NMe_2)$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000002	-0.000001	0.000005
2	H	-0.000006	-0.000004	-0.000002
3	P	-0.000076	0.000039	-0.000037
4	H	0.000009	0.000002	-0.000005
5	H	0.000001	-0.000001	0.000008
6	C	-0.000181	-0.000001	0.000313
7	O	0.000034	-0.000020	0.000169
8	C	0.000041	0.000231	0.000025
9	H	-0.000002	0.000003	-0.000016
10	H	-0.000001	0.000007	0.000017
11	C	-0.000063	0.000060	-0.000287
12	H	-0.000033	0.000014	-0.000020
13	H	-0.000004	-0.000007	-0.000005
14	Ni	0.000101	-0.000089	-0.000117
15	O	0.000086	0.000042	-0.000150
16	O	-0.000060	-0.000167	0.000014
17	H	0.000009	0.000004	-0.000004
18	C	0.000114	0.000044	-0.000007
19	C	0.000035	-0.000050	0.000047
20	C	-0.000001	0.000006	-0.000003
21	C	0.000001	0.000025	-0.000027
22	C	0.000010	-0.000016	0.000039
23	C	-0.000046	-0.000004	-0.000003
24	C	-0.000004	0.000008	0.000072
25	C	-0.000055	-0.000066	0.000007
26	C	0.000003	0.000023	-0.000037
27	C	0.000028	0.000015	0.000021
28	C	-0.000029	-0.000022	0.000005
29	C	0.000024	0.000018	-0.000011
30	H	0.000018	0.000024	-0.000003
31	N	0.000090	-0.000135	0.000022
32	C	0.000008	0.000049	-0.000037
33	H	-0.000012	-0.000005	0.000002
34	H	-0.000014	-0.000001	0.000001
35	H	0.000012	-0.000016	0.000011
36	C	-0.000018	0.000001	0.000010
37	H	-0.000014	0.000013	-0.000013
38	H	0.000000	-0.000004	0.000009
39	H	-0.000008	-0.000019	-0.000013

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23 $PPh_2(OEt)$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000063	-0.000106	0.000042
2	O	0.000163	-0.000237	-0.000130
3	P	0.000313	0.000262	0.000190
4	O	-0.000095	-0.000090	0.000154
5	O	-0.000052	-0.000011	-0.000005
6	C	-0.000176	0.000248	0.000123
7	C	0.000090	0.000130	-0.000218
8	C	0.000083	-0.000014	0.000026
9	C	0.000851	-0.000410	0.000675
10	H	0.000005	0.000004	0.000051
11	H	-0.000517	-0.000106	0.000868
12	H	0.000011	-0.000033	-0.000044
13	H	-0.000157	0.000057	-0.000008
14	H	-0.000012	0.000011	-0.000003
15	O	-0.000641	0.000276	-0.000693
16	C	0.000038	-0.000054	0.000000
17	C	-0.000033	-0.000005	0.000016
18	C	0.000015	0.000015	-0.000014
19	C	-0.000003	0.000002	0.000017
20	C	-0.000001	-0.000029	-0.000009
21	C	-0.000010	0.000047	0.000029
22	H	-0.000001	0.000010	0.000016
23	H	-0.000003	0.000001	0.000001
24	H	-0.000005	-0.000011	-0.000002
25	H	-0.000006	-0.000014	-0.000011
26	C	-0.000073	0.000097	-0.000047
27	C	0.000008	-0.000035	0.000028

28	C	-0.000041	0.000031	-0.000009
29	C	0.000017	0.000012	0.000008
30	C	-0.000016	0.000026	-0.000008
31	C	0.000059	-0.000070	0.000043
32	H	-0.000008	-0.000002	0.000023
33	H	0.000003	0.000000	0.000004
34	H	0.000004	-0.000005	0.000012
35	H	0.000000	-0.000004	-0.000002
36	C	-0.000265	-0.000022	-0.000451
37	H	0.000741	-0.000592	-0.000074
38	H	-0.000350	0.000620	-0.000600

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24 $P(tBu)_3$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000043	-0.000039	-0.000054
2	H	0.000038	0.000005	-0.000009
3	P	0.000392	-0.000428	0.000523
4	H	0.000001	0.000036	0.000017
5	H	-0.000053	0.000003	-0.000009
6	H	-0.000096	0.000089	-0.000003
7	H	0.000044	0.000064	-0.000018
8	H	-0.000017	-0.000006	-0.000009
9	C	0.000160	0.000227	0.000022
10	C	-0.000046	-0.000049	0.000136
11	C	0.000001	-0.000044	-0.000208
12	H	0.000101	-0.000105	-0.000037
13	H	0.000053	0.000073	-0.000015
14	Ni	-0.000633	0.000646	-0.000878
15	O	0.000371	-0.000188	-0.000303
16	O	-0.000565	-0.000143	0.000114
17	O	0.000590	0.000572	0.000467
18	C	-0.000360	0.000084	0.000378
19	C	0.000813	0.000157	-0.000063
20	C	-0.000424	-0.000606	-0.000229
21	C	-0.000218	-0.000084	0.000091
22	H	0.000080	-0.000031	-0.000022
23	H	0.000054	-0.000053	-0.000020
24	C	-0.000286	-0.000129	0.000043
25	H	0.000009	0.000075	-0.000001
26	H	0.000102	0.000068	-0.000016
27	C	-0.000026	0.000121	0.000084
28	H	0.000018	-0.000069	0.000059
29	H	0.000037	-0.000058	-0.000048
30	C	-0.000020	0.000098	0.000166
31	H	-0.000031	-0.000039	-0.000068
32	H	0.000035	-0.000064	-0.000009
33	C	0.000087	-0.000203	0.000153
34	H	-0.000029	0.000073	-0.000088
35	H	-0.000011	0.000078	0.000046
36	C	0.000217	0.000011	0.000066
37	H	-0.000094	-0.000025	-0.000003
38	H	-0.000048	0.000014	-0.000111
39	C	0.000076	-0.000002	-0.000035
40	H	-0.000058	0.000040	0.000019
41	H	0.000051	-0.000035	-0.000018
42	C	-0.000369	0.000015	-0.000280
43	H	0.000082	-0.000041	0.000033
44	H	0.000019	-0.000125	0.000106
45	C	0.000000	-0.000048	0.000080
46	H	-0.000077	0.000034	-0.000022
47	H	-0.000014	0.000032	-0.000028

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25 $PPh_2(Bn)$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000023	-0.000035	0.000039
2	H	0.000038	0.000002	0.000063
3	P	0.000014	0.000204	0.000009
4	H	-0.000037	0.000014	0.000027
5	H	0.000059	-0.000261	-0.000208
6	C	0.000054	-0.000106	-0.000107
7	O	0.000041	0.000087	0.000122
8	C	-0.000017	-0.000096	-0.000095
9	H	0.000008	-0.000001	0.000006
10	C	-0.000014	-0.000097	-0.000068
11	C	-0.000023	-0.000096	-0.000157
12	H	0.000272	-0.000315	-0.000024
13	H	-0.000012	-0.000013	-0.000012
14	Ni	-0.000024	0.000067	0.000092
15	O	-0.000048	0.000079	0.000059
16	O	0.000009	0.000086	0.000075
17	H	0.000003	0.000022	-0.000002
18	C	-0.000223	0.000015	0.000214
19	C	-0.000155	0.000341	0.000007
20	C	-0.000034	0.000003	0.000017
21	C	-0.000059	0.000038	-0.000049
22	C	0.000017	0.000018	-0.000004
23	C	0.000038	-0.000056	-0.000013
24	C	0.000012	0.000023	-0.000033
25	C	0.000002	0.000070	0.000029
26	C	-0.000013	-0.000089	-0.000036
27	C	0.000001	0.000011	0.000009
28	C	0.000008	0.000067	0.000032
29	C	-0.000011	-0.000082	-0.000026
30	H	-0.000004	-0.000027	-0.000005
31	H	0.000008	0.000028	0.000005
32	H	-0.000001	-0.000005	-0.000005
33	H	0.000005	-0.000013	-0.000009
34	H	-0.000013	0.000011	0.000008
35	C	-0.000060	0.000087	0.000027
36	C	-0.000006	-0.000055	0.000067
37	C	0.000058	0.000016	0.000018
38	C	-0.000025	-0.000001	-0.000005
39	C	0.000004	0.000002	0.000011
40	C	0.000125	0.000059	-0.000034
41	H	0.000002	-0.000014	-0.000032
42	H	-0.000032	0.000015	-0.000005
43	H	0.000016	-0.000005	-0.000022
44	H	-0.000006	0.000002	0.000014

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26 $PPh(Bn)_2$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000005	-0.000012	0.000026
2	H	0.000015	0.000038	0.000005
3	P	-0.000070	-0.000009	0.000083
4	H	0.000012	0.000006	-0.000016
5	H	0.000035	-0.000030	-0.000015
6	C	0.000082	-0.000132	0.000026
7	O	-0.000200	-0.000078	-0.000057
8	C	-0.000138	-0.000095	0.000105
9	C	0.000058	0.000116	-0.000128
10	C	-0.000096	-0.000012	0.000028
11	C	0.000221	0.000038	0.000025
12	H	-0.000012	0.000021	0.000013
13	H	-0.000014	-0.000009	0.000018
14	Ni	0.000128	0.000086	-0.000103
15	O	-0.000028	0.000058	0.000004

16	O	0.000063	0.000065	-0.000066
17	H	-0.000018	0.000002	0.000003
18	C	-0.000056	-0.000009	0.000017
19	C	-0.000010	-0.000027	-0.000064
20	C	-0.000005	-0.000014	0.000044
21	C	0.000000	0.000004	0.000000
22	C	0.000012	0.000013	0.000003
23	C	0.000022	-0.000004	0.000001
24	H	0.000017	-0.000002	0.000018
25	H	0.000012	0.000003	-0.000008
26	H	-0.000006	0.000009	0.000000
27	H	-0.000002	-0.000004	-0.000005
28	C	0.000024	-0.000046	-0.000018
29	C	-0.000053	0.000021	0.000042
30	C	0.000029	-0.000013	-0.000007
31	C	0.000031	0.000001	-0.000027
32	C	-0.000012	0.000000	0.000028
33	C	-0.000013	0.000005	-0.000018
34	H	0.000023	0.000002	0.000014
35	H	-0.000004	0.000002	0.000002
36	H	-0.000011	-0.000006	0.000009
37	H	-0.000005	0.000000	-0.000008
38	C	0.000007	0.000025	0.000016
39	C	0.000022	0.000012	0.000047
40	C	-0.000034	-0.000010	-0.000003
41	C	0.000015	0.000001	-0.000020
42	C	0.000017	-0.000001	0.000015
43	C	-0.000054	-0.000017	-0.000010
44	H	-0.000008	0.000003	-0.000028
45	H	0.000011	-0.000003	-0.000004
46	H	-0.000005	0.000006	0.000003
47	H	0.000002	-0.000002	0.000007

27 **P(OEt)3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000247	0.000111	0.000072
2	O	-0.000367	0.000059	0.000042
3	P	-0.000197	0.000005	-0.000146
4	O	-0.000319	-0.000551	-0.000016
5	O	0.000038	0.000405	0.000728
6	C	0.000250	-0.000042	0.000018
7	C	0.000289	0.000419	-0.000007
8	C	-0.000122	-0.000439	-0.000835
9	H	0.000007	0.000009	0.000007
10	H	0.000023	0.000051	0.000088
11	H	0.000062	0.000051	-0.000010
12	O	-0.000085	0.000001	0.000249
13	C	-0.000024	-0.000019	-0.000084
14	H	0.000011	0.000014	0.000001
15	H	0.000021	0.000015	-0.000002
16	O	-0.000060	-0.000101	0.000017
17	C	0.000027	-0.000057	-0.000065
18	H	0.000033	-0.000014	0.000005
19	H	-0.000025	0.000033	0.000018
20	O	0.000435	-0.000002	-0.000027
21	C	-0.000317	-0.000138	-0.000177
22	H	0.000007	-0.000014	0.000027
23	H	0.000064	0.000017	-0.000003
24	C	0.000082	0.000228	-0.000053
25	H	0.000049	0.000054	0.000006
26	H	0.000097	-0.000046	0.000044
27	C	-0.000050	-0.000027	-0.000023
28	H	0.000024	0.000026	0.000019
29	H	0.000019	-0.000007	0.000012
30	C	-0.000332	-0.000037	0.000149
31	H	0.000074	-0.000011	-0.000036
32	H	0.000042	0.000010	-0.000018

28 **P(*p*-tolyl)3**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000082	-0.000064	-0.000166
2	H	0.000130	0.000006	0.000091
3	P	-0.000070	0.000092	-0.000088
4	H	0.000024	0.000019	0.000041
5	H	-0.000050	0.000000	0.000006
6	C	-0.000051	0.000093	0.000139
7	O	0.000147	0.000108	0.000052
8	C	0.000253	0.000135	-0.000120
9	H	0.000023	0.000047	-0.000016
10	H	-0.000033	0.000036	-0.000042
11	C	-0.000155	-0.000105	-0.000081
12	H	-0.000006	0.000027	0.000017
13	H	0.000031	-0.000038	-0.000032
14	Ni	0.000005	-0.000057	0.000011
15	O	0.000054	-0.000110	-0.000127
16	O	-0.000192	-0.000101	0.000115
17	H	-0.000027	-0.000027	0.000001
18	C	0.000076	-0.000021	-0.000061
19	C	-0.000034	-0.000044	-0.000100
20	C	-0.000108	0.000131	-0.000050
21	C	0.000462	0.000148	0.000263
22	C	-0.000102	-0.000181	0.000082
23	C	-0.000012	0.000059	0.000036
24	C	0.000013	0.000061	0.000055
25	C	-0.000061	0.000077	0.000022
26	C	0.000135	0.000025	-0.000071
27	C	-0.000128	-0.000181	0.000508
28	C	-0.000095	-0.000112	-0.000197
29	C	0.000053	0.000010	0.000043
30	H	0.000016	0.000000	-0.000011
31	C	-0.000075	-0.000055	0.000003
32	C	0.000035	-0.000038	0.000075
33	C	0.000111	0.000193	-0.000093
34	C	0.000157	-0.000489	-0.000145
35	C	0.000010	0.000033	0.000137
36	C	-0.000099	-0.000005	-0.000045
37	H	-0.000017	0.000040	-0.000034
38	H	-0.000021	-0.000041	0.000023
39	H	0.000207	0.000033	-0.000034
40	H	-0.000025	-0.000004	-0.000051
41	H	-0.000001	0.000012	0.000024
42	C	-0.000167	0.000224	0.000064
43	H	-0.000007	-0.000091	0.000132
44	H	-0.000148	0.000006	-0.000120
45	C	0.000055	0.000181	-0.000233
46	H	-0.000118	0.000148	0.000010
47	H	-0.000029	-0.000206	-0.000047
48	C	-0.000219	-0.000052	-0.000211
49	H	-0.000013	0.000158	0.000021
50	H	-0.000015	-0.000081	0.000203

29 **P(vinyl)$_3$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	0.000140	-0.000091	-0.000018
2	C	-0.000161	0.000099	0.000123
3	O	-0.000083	0.000084	-0.000013
4	C	0.000027	0.000109	0.000174
5	O	0.000069	-0.000078	-0.000079
6	O	0.000019	-0.000132	-0.000148
7	Ni	-0.000068	-0.000018	0.000031
8	P	0.000029	-0.000029	0.000086
9	H	-0.000001	-0.000096	0.000018

10	H	-0.000096	0.000008	-0.000050
11	H	0.000025	0.000032	-0.000068
12	C	-0.000059	-0.000077	0.000021
13	H	-0.000013	0.000009	0.000047
14	C	-0.000098	-0.000008	-0.000034
15	H	0.000007	-0.000019	0.000078
16	C	-0.000008	0.000137	-0.000049
17	H	0.000090	-0.000022	0.000048
18	C	-0.000030	-0.000026	0.000011
19	H	0.000075	0.000007	0.000037
20	C	0.000139	-0.000057	-0.000080
21	H	-0.000023	0.000065	-0.000041
22	C	0.000021	0.000019	-0.000088
23	H	-0.000003	0.000085	-0.000007

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30 **$PPh_2(p\text{-}C_6H_4F)$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	F	-0.000166	-0.000053	-0.000018
2	H	-0.000002	0.000002	-0.000001
3	P	0.000133	0.000222	-0.000071
4	H	-0.000004	-0.000005	0.000002
5	H	0.000000	0.000001	0.000001
6	C	-0.000024	0.000054	0.000082
7	O	0.000063	0.000047	0.000040
8	C	0.000041	0.000026	-0.000061
9	H	-0.000057	0.000002	-0.000018
10	H	-0.000002	-0.000004	-0.000019
11	C	-0.000081	-0.000047	-0.000038
12	H	0.000043	-0.000008	-0.000010
13	H	-0.000051	-0.000033	-0.000011
14	Ni	0.000129	-0.000079	0.000083
15	O	0.000024	-0.000066	-0.000099
16	O	-0.000059	-0.000027	0.000086
17	H	0.000038	0.000041	0.000002
18	C	-0.000210	-0.000082	-0.000050
19	C	-0.000075	0.000036	0.000015
20	C	0.000094	0.000066	0.000031
21	C	0.000124	0.000034	0.000000
22	C	0.000114	0.000011	0.000002
23	C	-0.000054	-0.000071	0.000048
24	C	-0.000037	-0.000044	0.000004
25	C	0.000003	0.000059	-0.000005
26	C	0.000011	-0.000022	0.000011
27	C	-0.000005	0.000003	-0.000009
28	C	0.000003	0.000006	-0.000005
29	C	0.000008	0.000009	0.000036
30	H	0.000007	-0.000024	-0.000003
31	C	0.000015	-0.000033	-0.000056
32	C	0.000018	-0.000012	0.000006
33	C	-0.000023	0.000004	0.000011
34	C	0.000017	0.000014	-0.000008
35	C	-0.000029	-0.000031	0.000000
36	C	-0.000016	0.000007	0.000018
37	H	-0.000008	-0.000003	-0.000001
38	H	0.000016	-0.000001	-0.000001
39	H	0.000000	-0.000001	0.000000
40	H	0.000012	0.000001	0.000001
41	H	-0.000009	-0.000001	0.000006

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31 **$PPh_2(OPh)$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000002	0.000000	0.000002
2	H	-0.000076	-0.000147	-0.000003
3	P	-0.000095	0.000260	0.000173
4	H	-0.000006	0.000009	-0.000006
5	H	0.000011	-0.000006	-0.000001
6	C	-0.000002	0.000102	0.000064
7	O	0.000068	-0.000017	0.000002
8	C	-0.000032	-0.000081	0.000121
9	H	0.000001	0.000019	-0.000006
10	O	-0.000053	-0.000174	0.000172
11	C	-0.000073	0.000058	-0.000017
12	H	-0.000213	0.000261	0.000050
13	H	0.000007	-0.000012	0.000013
14	Ni	-0.000058	-0.000016	-0.000039
15	O	0.000045	-0.000121	-0.000060
16	O	0.000048	0.000072	-0.000141
17	H	0.000005	0.000016	-0.000020
18	C	0.000095	0.000048	-0.000111
19	C	0.000051	-0.000153	0.000042
20	C	-0.000044	0.000058	-0.000005
21	C	-0.000020	-0.000032	0.000015
22	C	0.000102	0.000004	0.000013
23	C	-0.000011	-0.000094	0.000000
24	C	0.000078	-0.000004	0.000018
25	C	0.000004	0.000024	0.000031
26	C	-0.000001	0.000022	-0.000018
27	C	-0.000002	-0.000052	-0.000015
28	C	0.000005	0.000052	0.000044
29	C	0.000003	0.000036	0.000021
30	H	-0.000015	-0.000016	-0.000024
31	H	-0.000001	-0.000004	-0.000001
32	H	0.000000	0.000004	0.000001
33	H	-0.000009	-0.000023	-0.000016
34	H	-0.000008	-0.000012	-0.000007
35	C	0.000172	-0.000129	-0.000193
36	C	-0.000025	-0.000007	0.000022
37	C	-0.000038	0.000011	-0.000049
38	C	0.000058	-0.000047	0.000018
39	C	-0.000039	0.000031	-0.000060
40	C	0.000073	0.000064	-0.000021
41	H	0.000007	-0.000006	-0.000012
42	H	-0.000012	0.000003	0.000003

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32 **$PPh_2(vinyl)$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000005	0.000009	0.000000
2	H	-0.000001	-0.000010	-0.000002
3	P	0.000219	-0.000107	0.000122
4	H	-0.000004	0.000001	0.000001
5	H	0.000001	-0.000001	0.000007
6	C	0.000061	-0.000092	-0.000027
7	O	-0.000069	0.000031	0.000028
8	C	-0.000006	-0.000121	0.000091
9	H	0.000005	0.000003	-0.000006
10	H	-0.000015	0.000025	0.000003
11	C	0.000113	-0.000056	-0.000030
12	H	-0.000004	0.000004	0.000020
13	H	-0.000005	-0.000002	0.000003
14	Ni	-0.000254	0.000238	-0.000176
15	O	-0.000051	0.000096	0.000010
16	O	0.000007	0.000107	-0.000064
17	H	-0.000008	-0.000001	0.000018
18	C	0.000003	-0.000020	0.000039
19	C	0.000027	-0.000009	-0.000034
20	C	-0.000004	-0.000008	0.000004
21	C	-0.000005	0.000007	-0.000004
22	C	-0.000002	-0.000015	-0.000005
23	C	-0.000010	0.000003	-0.000027

24	C	-0.000041	-0.000050	0.000005
25	C	0.000003	0.000037	0.000002
26	C	-0.000019	-0.000003	0.000001
27	C	-0.000024	0.000006	0.000015
28	C	0.000028	0.000004	-0.000014
29	C	0.000008	-0.000021	0.000013
30	H	0.000008	-0.000006	0.000004
31	H	0.000012	0.000002	-0.000005
32	C	-0.000018	0.000091	0.000001
33	H	0.000008	-0.000052	0.000014
34	C	0.000029	-0.000111	-0.000039
35	H	0.000012	0.000021	0.000032

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33 **P(p-$C_6H_4Cl)_3$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Cl	-0.000007	-0.000037	-0.000019
2	Cl	-0.000091	-0.000061	0.000251
3	P	0.000169	-0.000135	0.000064
4	H	-0.000090	-0.000012	0.000031
5	H	0.000034	0.000005	0.000006
6	C	0.000376	-0.000352	-0.000167
7	O	-0.000869	-0.000783	-0.000522
8	C	0.000505	0.000137	-0.000826
9	H	-0.000002	-0.000026	0.000002
10	H	0.000078	0.000015	-0.000181
11	C	0.000713	0.000798	0.000591
12	H	-0.000106	-0.000035	-0.000001
13	H	-0.000017	0.000017	-0.000003
14	Ni	-0.000107	0.000134	0.000064
15	O	-0.000236	0.000339	0.000111
16	O	-0.000533	-0.000176	0.000748
17	H	-0.000090	-0.000104	-0.000037
18	C	-0.000206	0.000249	0.000103
19	C	0.000197	-0.000074	0.000011
20	C	-0.000045	-0.000199	-0.000046
21	C	0.000083	0.000155	0.000030
22	C	-0.000082	-0.000008	0.000069
23	C	0.000108	0.000092	-0.000038
24	C	0.000171	0.000062	-0.000072
25	C	-0.000206	0.000005	0.000229
26	C	-0.000219	0.000066	-0.000190
27	C	0.000239	0.000046	-0.000099
28	C	0.000155	-0.000007	-0.000017
29	C	-0.000240	-0.000059	0.000032
30	H	0.000136	-0.000014	-0.000051
31	C	0.000069	0.000172	-0.000101
32	C	-0.000010	-0.000299	-0.000063
33	C	-0.000001	0.000078	0.000325
34	C	0.000083	0.000237	0.000031
35	C	0.000000	0.000174	-0.000053
36	C	0.000144	-0.000187	-0.000063
37	H	-0.000020	0.000133	-0.000026
38	H	-0.000005	-0.000001	-0.000063
39	Cl	-0.000054	-0.000383	-0.000186
40	H	-0.000006	-0.000047	0.000031
41	H	-0.000020	0.000088	0.000095

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34 **P(p-$C_6H_4F)_3$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	F	-0.000010	-0.000013	0.000033
2	F	0.000029	0.000003	-0.000100
3	P	-0.000006	0.000434	-0.000249
4	H	-0.000059	-0.000018	0.000018
5	H	0.000033	-0.000011	0.000059
6	C	0.000027	0.000218	0.000013
7	O	0.000040	-0.000033	0.000079
8	C	-0.000044	0.000172	-0.000022
9	H	0.000000	0.000000	-0.000003
10	H	0.000008	-0.000039	-0.000054
11	C	-0.000072	0.000034	-0.000084
12	H	0.000015	0.000000	-0.000007
13	H	0.000006	0.000005	0.000000
14	Ni	0.000201	-0.000285	0.000199
15	O	-0.000049	-0.000116	0.000036
16	O	0.000023	-0.000117	-0.000001
17	H	-0.000016	-0.000025	-0.000011
18	C	-0.000122	-0.000015	-0.000056
19	C	0.000063	-0.000026	0.000150
20	C	-0.000047	-0.000079	0.000008
21	C	-0.000003	0.000092	-0.000080
22	C	0.000056	-0.000013	0.000036
23	C	0.000025	-0.000010	-0.000067
24	C	0.000038	-0.000081	0.000200
25	C	-0.000073	-0.000082	0.000014
26	C	-0.000033	0.000051	-0.000122
27	C	0.000029	-0.000048	0.000193
28	C	-0.000017	0.000056	-0.000029
29	C	-0.000040	0.000119	-0.000016
30	H	0.000027	-0.000022	-0.000020
31	C	-0.000025	-0.000200	-0.000103
32	C	-0.000009	0.000003	-0.000036
33	C	-0.000051	0.000044	0.000036
34	C	0.000073	-0.000180	-0.000044
35	C	-0.000030	0.000072	-0.000009
36	C	0.000010	-0.000009	-0.000033
37	H	0.000003	0.000050	0.000024
38	H	0.000012	-0.000017	-0.000058
39	F	-0.000019	0.000108	0.000037
40	H	0.000008	-0.000058	0.000031
41	H	0.000000	0.000036	0.000042

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35 **PPh$(OPh)_2$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000077	0.000032	-0.000024
2	H	-0.000043	-0.000016	0.000010
3	P	-0.000078	-0.000413	0.000586
4	H	-0.000002	-0.000007	-0.000033
5	H	-0.000065	0.000006	-0.000018
6	C	-0.000294	-0.000026	-0.000104
7	O	-0.000192	-0.000240	-0.000032
8	C	0.000053	-0.000220	0.000102
9	O	-0.000030	0.000171	-0.000299
10	O	0.000087	0.000122	-0.000319
11	C	0.000489	0.000431	0.000069
12	H	-0.000022	-0.000044	-0.000031
13	H	0.000008	0.000015	0.000007
14	Ni	-0.000269	-0.000123	-0.000543
15	O	0.000197	0.000213	0.000279
16	O	-0.000105	0.000134	-0.000024
17	H	0.000004	-0.000021	-0.000001
18	C	0.000062	0.000019	0.000124
19	C	-0.000009	0.000044	-0.000057
20	C	0.000014	-0.000018	0.000049
21	C	-0.000010	0.000026	-0.000039
22	C	0.000040	-0.000060	-0.000034
23	C	0.000003	0.000079	-0.000015
24	H	0.000001	-0.000021	-0.000003
25	H	-0.000019	0.000002	-0.000017
26	H	-0.000004	-0.000007	0.000017

27	H	-0.000020	0.000009	0.000008
28	C	-0.000174	-0.000206	0.000175
29	C	-0.000085	0.000363	-0.000084
30	C	0.000138	-0.000127	-0.000185
31	C	-0.000093	-0.000012	0.000105
32	C	-0.000008	0.000050	0.000015
33	C	0.000213	-0.000079	0.000044
34	H	0.000050	-0.000155	0.000094
35	H	-0.000066	0.000041	0.000031
36	H	0.000030	0.000030	0.000001
37	H	0.000003	-0.000007	-0.000039
38	C	0.000258	0.000003	0.000208
39	C	-0.000219	-0.000038	-0.000011
40	C	0.000104	0.000055	0.000020
41	C	-0.000001	0.000025	-0.000011
42	C	0.000022	-0.000037	-0.000039
43	C	-0.000046	0.000010	0.000019

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36 $P(Bn)_3$ (Bn = benzyl)

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000012	0.000003	0.000001
2	H	0.000017	0.000026	0.000038
3	P	0.000019	-0.000083	0.000033
4	H	0.000022	0.000006	-0.000025
5	H	0.000001	0.000018	0.000027
6	H	0.000002	-0.000017	0.000001
7	H	-0.000009	0.000003	0.000003
8	H	0.000002	0.000021	-0.000015
9	C	-0.000012	-0.000000	0.000005
10	C	0.000018	-0.000001	-0.000006
11	C	0.000026	-0.000019	-0.000011
12	H	-0.000004	-0.000008	-0.000011
13	H	0.000001	-0.000000	-0.000003
14	Ni	-0.000061	0.000084	-0.000081
15	O	0.000019	0.000029	-0.000017
16	O	-0.000010	0.000004	0.000003
17	O	-0.000015	0.000026	0.000016
18	C	-0.000025	-0.000063	0.000018
19	C	-0.000006	-0.000017	0.000021
20	C	0.000041	-0.000039	-0.000001
21	C	-0.000006	0.000007	0.000014
22	C	-0.000006	-0.000002	0.000002
23	C	0.000002	0.000003	0.000000
24	C	0.000003	0.000001	-0.000007
25	C	0.000000	0.000002	0.000005
26	C	-0.000002	-0.000004	0.000011
27	H	0.000004	0.000002	-0.000003
28	H	0.000000	0.000001	-0.000002
29	H	-0.000002	-0.000000	0.000003
30	H	0.000000	0.000002	-0.000002
31	C	-0.000029	0.000061	0.000036
32	C	0.000018	-0.000017	0.000008
33	C	-0.000000	-0.000030	-0.000004
34	C	-0.000019	0.000025	0.000026
35	C	0.000014	-0.000005	-0.000022
36	C	0.000021	0.000004	0.000009
37	H	-0.000009	-0.000036	-0.000021
38	H	0.000001	0.000010	-0.000006
39	H	-0.000001	-0.000007	-0.000009
40	H	-0.000001	-0.000001	-0.000002
41	C	-0.000007	-0.000003	-0.000003
42	C	-0.000009	0.000001	0.000012
43	C	-0.000004	0.000011	0.000004
44	C	0.000005	-0.000005	-0.000012
45	C	-0.000003	0.000006	0.000013
46	C	0.000000	-0.000001	-0.000040
47	H	-0.000000	-0.000001	-0.000000
48	H	-0.000004	0.000001	-0.000000
49	H	-0.000001	-0.000001	-0.000002
50	H	-0.000002	0.000004	-0.000002

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37 $P(tBu)_2F$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000209	0.000102	-0.000334
2	O	0.000223	-0.000201	-0.000192
3	P	0.000143	0.000072	0.000013
4	O	-0.000828	-0.000770	0.000581
5	O	0.000244	0.000238	-0.000154
6	C	-0.000345	0.000294	0.000309
7	C	0.000650	0.000651	-0.000495
8	C	-0.000282	-0.000250	0.000282
9	H	-0.000067	-0.000025	0.000022
10	F	-0.000024	-0.000125	-0.000002
11	H	0.000006	0.000025	0.000009
12	C	0.000062	0.000059	-0.000194
13	C	0.000050	-0.000173	0.000063
14	H	-0.000010	0.000048	0.000001
15	H	0.000017	0.000007	-0.000040
16	H	-0.000039	0.000020	0.000018
17	C	-0.000099	0.000152	0.000018
18	H	-0.000071	-0.000044	0.000035
19	H	-0.000002	-0.000019	0.000015
20	H	0.000050	-0.000021	-0.000046
21	C	-0.000038	-0.000103	0.000063
22	H	-0.000002	0.000001	0.000011
23	H	-0.000024	0.000007	0.000014
24	C	-0.000035	-0.000015	0.000269
25	C	-0.000027	0.000028	-0.000090
26	H	0.000043	-0.000016	-0.000002
27	H	0.000049	0.000015	0.000029
28	H	0.000040	-0.000027	-0.000001
29	C	-0.000027	-0.000042	-0.000165
30	H	-0.000013	0.000034	-0.000011
31	H	0.000003	0.000034	-0.000006
32	H	0.000023	0.000003	0.000017
33	C	0.000160	0.000072	-0.000171
34	H	-0.000036	-0.000004	0.000049
35	H	-0.000002	-0.000024	0.000088

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38 $P(^tBu)F_2$

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	Ni	0.000034	0.000040	-0.000102
2	O	0.000001	-0.000013	0.000008
3	P	0.000039	-0.000002	0.000050
4	O	0.000002	0.000019	-0.000035
5	O	0.000070	0.000014	-0.000083
6	C	-0.000033	0.000041	0.000028
7	C	0.000013	-0.000050	0.000024
8	C	-0.000101	-0.000032	0.000123
9	F	-0.000005	0.000000	0.000009
10	F	0.000005	0.000008	-0.000011
11	H	0.000001	-0.000005	-0.000007
12	C	-0.000053	0.000014	0.000021
13	C	0.000024	-0.000041	-0.000029
14	H	-0.000011	0.000002	0.000008
15	H	0.000003	0.000003	0.000002
16	H	-0.000010	-0.000003	-0.000001
17	C	0.000012	0.000003	0.000007
18	H	0.000001	-0.000005	-0.000004
19	H	-0.000002	-0.000003	-0.000002

20	H	0.000000	-0.000003	0.000004
21	C	0.000015	0.000018	0.000004
22	H	-0.000004	-0.000001	-0.000002
23	H	0.000002	-0.000005	-0.000012

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39 **P(^{n}Bu)$_3$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000101	0.000001	-0.000090
2	H	0.000060	-0.000032	-0.000085
3	P	0.000116	-0.000024	-0.000292
4	H	0.000121	0.000000	-0.000225
5	H	0.000024	0.000002	-0.000015
6	H	0.000058	-0.000010	-0.000045
7	H	-0.000023	-0.000082	0.000024
8	H	0.000025	-0.000037	0.000129
9	C	-0.000165	0.000105	0.000205
10	C	0.000048	0.000220	0.000349
11	C	0.000069	0.000271	-0.000278
12	H	0.000015	0.000010	-0.000040
13	H	0.000010	-0.000001	0.000001
14	Ni	-0.000520	-0.000131	0.001330
15	O	-0.000280	0.000567	0.000402
16	O	0.001219	0.000391	-0.001053
17	O	0.000725	0.000493	0.001451
18	C	0.000370	-0.000467	-0.000559
19	C	-0.001205	-0.000547	0.001022
20	C	-0.000409	-0.000698	-0.001919
21	C	-0.000028	0.000013	0.000138
22	H	-0.000048	0.000052	-0.000310
23	H	0.000030	0.000001	-0.000020
24	C	-0.000017	0.000131	-0.000030
25	H	0.000051	-0.000051	-0.000062
26	H	0.000042	0.000004	0.000030
27	C	-0.000007	0.000003	0.000027
28	H	0.000011	0.000034	-0.000027
29	H	0.000034	-0.000004	-0.000013
30	C	-0.000013	-0.000317	-0.000054
31	H	0.000027	0.000026	-0.000066
32	H	0.000007	0.000003	-0.000022
33	C	0.000084	0.000142	0.000179
34	H	0.000028	0.000038	-0.000030
35	H	-0.000074	-0.000078	0.000062
36	C	-0.000061	-0.000188	0.000009
37	H	-0.000051	-0.000017	0.000029
38	H	-0.000001	-0.000002	-0.000005
39	C	-0.000081	0.000010	-0.000173
40	H	-0.000027	-0.000037	0.000084
41	H	-0.000110	-0.000021	0.000044
42	C	-0.000005	-0.000036	-0.000003
43	H	0.000043	0.000028	-0.000013
44	H	0.000006	0.000142	0.000028
45	C	0.000047	0.000079	-0.000160
46	H	-0.000011	0.000016	0.000029
47	H	-0.000031	0.000001	0.000016

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40 **P(*p*-C$_6$H$_4$-OMe)$_3$**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	0.000005	0.000002	0.000006
2	H	0.000014	0.000006	-0.000016
3	P	0.000241	-0.000065	0.000217
4	H	-0.000001	-0.000006	0.000008
5	H	-0.000001	-0.000008	0.000010
6	C	0.000095	-0.000001	0.000096
7	O	-0.000170	-0.000005	0.000060
8	C	-0.000019	-0.000035	0.000110
9	H	-0.000009	-0.000003	-0.000005
10	H	0.000000	0.000011	0.000017
11	C	0.000149	-0.000058	-0.000043
12	H	0.000011	-0.000012	-0.000028
13	H	0.000015	0.000006	-0.000004
14	Ni	-0.000143	0.000146	-0.000287
15	O	-0.000051	0.000037	-0.000056
16	O	-0.000006	0.000033	-0.000007
17	H	0.000012	-0.000008	-0.000001
18	C	-0.000011	-0.000080	0.000123
19	C	-0.000054	-0.000010	0.000012
20	C	0.000005	0.000036	-0.000044
21	C	-0.000045	0.000026	0.000081
22	C	0.000018	0.000003	-0.000012
23	C	0.000009	-0.000022	-0.000070
24	C	-0.000038	0.000065	-0.000038
25	C	0.000013	-0.000029	-0.000074
26	C	-0.000019	-0.000032	0.000018
27	C	0.000058	0.000064	0.000027
28	C	0.000006	-0.000012	-0.000021
29	C	0.000012	-0.000050	0.000006
30	H	0.000002	-0.000004	-0.000006
31	C	-0.000219	0.000037	-0.000078
32	C	0.000040	-0.000057	0.000002
33	C	0.000007	0.000022	0.000045
34	C	0.000000	-0.000009	-0.000027
35	C	0.000014	-0.000015	-0.000026
36	C	0.000064	0.000021	0.000003
37	H	0.000010	0.000006	-0.000005
38	H	0.000009	-0.000007	-0.000017
39	H	-0.000007	0.000014	0.000010
40	H	0.000005	0.000019	0.000019
41	H	-0.000001	-0.000021	-0.000010
42	O	-0.000017	0.000004	0.000011
43	C	0.000005	0.000017	0.000002
44	H	0.000002	0.000003	0.000003
45	H	-0.000003	-0.000018	-0.000007
46	O	-0.000017	-0.000001	-0.000002
47	C	-0.000019	0.000007	0.000011
48	H	-0.000003	-0.000004	-0.000009
49	H	-0.000002	-0.000004	0.000012
50	O	0.000022	-0.000002	-0.000005
51	C	0.000016	-0.000003	-0.000014
52	H	0.000000	-0.000002	0.000003
53	H	-0.000007	-0.000001	0.000003

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41 **PPh$_2$(*p*-C$_6$H$_4$-OMe)**

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	-0.000169	0.000363	0.000017
2	H	0.000003	0.000001	-0.000008
3	P	-0.000040	0.000174	0.000189
4	H	-0.000002	-0.000004	-0.000001
5	H	0.000006	0.000010	0.000007
6	C	0.000087	0.000166	-0.000087
7	O	-0.000054	-0.000098	-0.000040
8	C	-0.000090	0.000224	-0.000213
9	H	0.000035	-0.000039	-0.000054
10	H	-0.000008	-0.000004	0.000002
11	C	0.000183	0.000169	0.000111
12	H	0.000009	0.000020	0.000065
13	H	0.000014	-0.000037	0.000005
14	Ni	-0.000061	-0.000234	-0.000017

15	O	-0.000059	-0.000113	0.000051
16	O	0.000043	-0.000136	0.000202
17	H	0.000022	0.000015	-0.000046
18	C	-0.000121	-0.000201	-0.000107
19	C	0.000229	-0.000100	-0.000074
20	C	0.000404	0.000037	0.000017
21	C	-0.000681	-0.000277	0.000010
22	C	0.000128	0.000223	0.000036
23	C	-0.000084	0.000169	0.000067
24	C	0.000110	-0.000098	-0.000008
25	C	0.000040	-0.000014	0.000012
26	C	0.000000	-0.000049	-0.000036
27	C	0.000016	0.000036	0.000034
28	C	-0.000044	-0.000043	0.000028
29	C	0.000023	0.000144	-0.000063
30	H	-0.000044	0.000033	-0.000020
31	C	-0.000054	0.000029	-0.000014
32	C	0.000044	-0.000060	-0.000009
33	C	-0.000111	0.000045	0.000059
34	C	0.000067	0.000013	-0.000090
35	C	0.000000	-0.000043	0.000028
36	C	0.000077	0.000006	-0.000031
37	H	-0.000026	0.000016	-0.000021
38	H	0.000014	-0.000008	-0.000018
39	H	-0.000005	-0.000006	0.000019
40	H	-0.000005	0.000018	-0.000008
41	H	-0.000062	-0.000041	0.000002
42	H	-0.000087	-0.000119	-0.000022
43	C	0.000294	0.000078	0.000082
44	H	-0.000023	-0.000135	-0.000029
45	H	-0.000016	-0.000129	-0.000026

#3 Table T1: Charge transfer magnitudes for complexes 1-41

#	Phosphine	Δq_1	Δq_2	Δq_3	Δq_4	Δq_σ^d	Δq_π^{bd}	Δq_σ^{bd}	Δq^{part}	Δq^{tot}
1	$P(C_6F_5)_3$	0.43557	0.27644	0.27021	0.18266	0.43557	0.54665	0.18266	-0.11108	-0.29374
2	$P(OMe)_3$	0.51451	0.27616	0.26199	0.16848	0.51451	0.53815	0.16848	-0.02364	-0.19212
3	$P(OMe)Ph_2$	0.53852	0.27267	0.24864	0.16866	0.53852	0.52131	0.16866	0.01721	-0.15145
4	$P(OPh)_3$	0.48558	0.29569	0.28672	0.15420	0.48558	0.58241	0.15420	-0.09683	-0.25103
5	PCl_2Ph	0.47476	0.32241	0.30686	0.16528	0.47476	0.62927	0.16528	-0.15451	-0.31979
6	PCl_3	0.44059	0.34974	0.34918	0.18392	0.44059	0.69892	0.18392	-0.25833	-0.44225
7	$PClPh_2$	0.50748	0.30300	0.25819	0.17038	0.50748	0.56119	0.17038	-0.05371	-0.22409
8	PEt_3	0.59198	0.22501	0.22473	0.16357	0.59198	0.44974	0.16357	0.14224	-0.02133
9	PF_3	0.43596	0.35334	0.35148	0.18235	0.43596	0.70482	0.18235	-0.26886	-0.45121
10	PH_2Ph	0.49545	0.25692	0.24377	0.16762	0.49545	0.50069	0.16762	-0.00524	-0.17286
11	$PHPh_2$	0.51450	0.24996	0.24285	0.16930	0.51450	0.49281	0.16930	0.02169	-0.14761
12	PMe_2CF_3	0.49338	0.28034	0.24082	0.16177	0.49338	0.52116	0.16177	-0.02778	-0.18955
13	PMe_2Ph	0.54751	0.23550	0.21756	0.15610	0.54751	0.45306	0.15610	0.09445	-0.06165
14	PMe_3	0.56056	0.22480	0.22440	0.16180	0.56056	0.44920	0.16180	0.11136	-0.05044
15	$PMePh_2$	0.54204	0.23880	0.22862	0.16918	0.54204	0.46742	0.16918	0.07462	-0.09456
16	$P(NMe_2)_3$	0.55458	0.23618	0.22447	0.14571	0.55458	0.46065	0.14571	0.09393	-0.05178
17	PPh_3	0.53130	0.23621	0.23304	0.17326	0.53130	0.46925	0.17326	0.06205	-0.11121
18	PEt_2Ph	0.54760	0.23208	0.21432	0.16371	0.54760	0.44640	0.16371	0.10120	-0.06251
19	$PEtPh_2$	0.54051	0.23552	0.22570	0.16518	0.54051	0.46122	0.16518	0.07929	-0.08589
20	$PPh(OEt)_2$	0.54205	0.27211	0.25630	0.16474	0.54205	0.52841	0.16474	0.01364	-0.15110
21	$PPh_2(C_6F_5)$	0.49866	0.25794	0.24406	0.17262	0.49866	0.50200	0.17262	-0.00334	-0.17596
22	$PPh_2(NMe_2)$	0.56269	0.24865	0.23459	0.15492	0.56269	0.48324	0.15492	0.07945	-0.07547
23	$PPh_2(OEt)$	0.53940	0.27042	0.24769	0.16837	0.53940	0.51811	0.16837	0.02129	-0.14708
24	$P(^tBu)_3$	0.53955	0.20898	0.20821	0.13399	0.53955	0.41719	0.13399	0.12236	-0.01163
25	$PPPh_2Bn$	0.54302	0.24020	0.22238	0.16761	0.54302	0.46258	0.16761	0.08044	-0.08717
26	$PPhBn_2$	0.53287	0.24175	0.22961	0.15738	0.53287	0.47136	0.15738	0.06151	-0.09587
27	$P(OEt)_3$	0.52254	0.27576	0.24709	0.16214	0.52254	0.52285	0.16214	-0.00031	-0.16245
28	$P(p\text{-tolyl})_3$	0.53956	0.23245	0.22923	0.17226	0.53956	0.46168	0.17226	0.07788	-0.09438
29	$P(vinyl)_3$	0.53970	0.23963	0.23833	0.19226	0.53970	0.47796	0.19226	0.06174	-0.13052

30	$PPh_2(C_6H_4F)$	0.52602	0.23883	0.23397	0.17153	0.52602	0.47280	0.17153	0.05322	-0.11831
31	$PPh_2(OPh)$	0.53279	0.28887	0.25065	0.16989	0.53279	0.53952	0.16989	-0.00673	-0.17662
32	PPh_2(vinyl)	0.53143	0.23726	0.23669	0.17792	0.53143	0.47395	0.17792	0.05748	-0.12044
33	$P(C_6H_4Cl)_3$	0.51602	0.24350	0.24122	0.17336	0.51602	0.48472	0.17336	0.03130	-0.14206
34	$P(C_6H_4F)_3$	0.51858	0.24030	0.23693	0.16946	0.51858	0.47723	0.16946	0.04135	-0.12811
35	$PPh(OPh)_2$	0.50682	0.29407	0.26803	0.15865	0.50682	0.56210	0.15865	-0.05528	-0.21393
36	P(benzyl)$_3$	0.52711	0.24139	0.23573	0.15631	0.52711	0.47712	0.15631	0.04999	-0.10632
37	$P(^tBu)_2F$	0.52863	0.28209	0.23824	0.14517	0.52863	0.52033	0.14517	0.00830	-0.13687
38	$P(^tBu)F_2$	0.49433	0.33263	0.30262	0.16923	0.49433	0.63525	0.16923	-0.14092	-0.31015
39	$P(^nBu)_3$	0.56527	0.22155	0.21336	0.15484	0.56527	0.43491	0.15484	0.13036	-0.02448
40	P(anis)$_3$	0.54329	0.22983	0.22410	0.16820	0.54329	0.45393	0.16820	0.08936	-0.07884
41	PPh_2(anis)	0.53520	0.23592	0.22901	0.17234	0.53520	0.46493	0.17234	0.07027	-0.10207

$\Delta q_\sigma^d = \Delta q_1$; $\Delta q_\pi^{bd} = \Delta q_2 + \Delta q_3$; $\Delta q_\sigma^{bd} = \Delta q_4$

$\Delta q^{part} = \Delta q_\sigma^d - \Delta q_\pi^{bd}$

$\Delta q^{tot} = \Delta q_\sigma^d - \Delta q_\pi^{bd} - \Delta q_\sigma^{bd}$

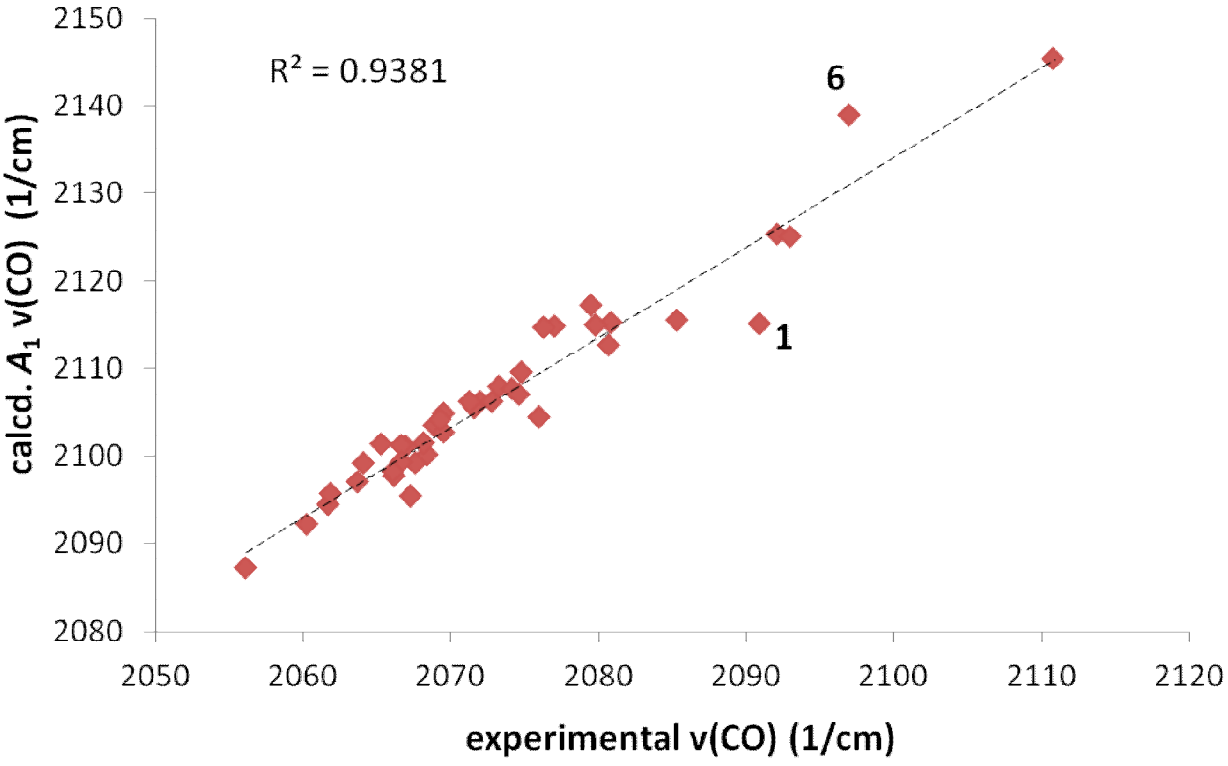
#4 Table T2: ETS-NOCV results for compounds 1-41

#	Phosphine	ΔE_1	ΔE_2	ΔE_3	ΔE_4	ΔE_{rest}	E_σ^d	E_π^{bd}	E_σ^{bd}
1	$P(C_6F_5)_3$	-16.42	-8.00	-7.70	-5.91	-1.95	-16.42	-15.70	-5.91
2	$P(OMe)_3$	-23.35	-8.98	-8.45	-6.17	-0.38	-23.35	-17.43	-6.17
3	$P(OMe)Ph_2$	-23.73	-8.42	-7.63	-5.73	-0.88	-23.73	-16.06	-5.73
4	$P(OPh)_3$	-21.03	-10.41	-9.61	-5.53	-1.25	-21.03	-20.02	-5.53
5	PCl_2Ph	-19.33	-10.45	-10.43	-6.39	-1.45	-19.33	-20.88	-6.39
6	PCl_3	-17.08	-12.37	-12.37	-7.53	-1.95	-17.08	-24.74	-7.53
7	$PClPh_2$	-21.19	-9.30	-8.10	-6.11	-1.21	-21.19	-17.39	-6.11
8	PEt_3	-28.03	-6.77	-6.79	-5.76	-0.63	-28.03	-13.56	-5.76
9	PF_3	-18.99	-15.36	-15.27	-8.19	-1.56	-18.99	-30.63	-8.19
10	PH_2Ph	-21.41	-7.91	-7.07	-5.89	-0.37	-21.41	-14.97	-5.89
11	$PHPh_2$	-22.18	-7.29	-7.28	-5.73	-0.80	-22.18	-14.57	-5.73
12	PMe_2CF_3	-21.09	-8.86	-7.42	-5.76	-0.73	-21.09	-16.28	-5.76
13	PMe_2Ph	-24.76	-7.06	-6.14	-5.12	-0.83	-24.76	-13.20	-5.12
14	PMe_3	-25.83	-6.51	-6.52	-5.43	-0.54	-25.83	-13.04	-5.43
15	$PMePh_2$	-23.73	-7.04	-6.56	-5.57	-1.10	-23.73	-13.59	-5.57
16	$P(NMe_2)_3$	-25.23	-7.09	-6.64	-4.57	-1.85	-25.23	-13.74	-4.57
17	PPh_3	-22.73	-6.81	-6.63	-5.61	-1.39	-22.73	-13.45	-5.61
18	PEt_2Ph	-24.03	-6.52	-5.86	-5.21	-1.03	-24.03	-12.38	-5.21
19	$PEtPh_2$	-23.78	-6.89	-6.46	-5.38	-1.34	-23.78	-13.35	-5.38
20	$PPh(OEt)_2$	-24.61	-8.85	-7.98	-5.76	-0.88	-24.61	-16.83	-5.76
21	$PPh_2(C_6F_5)$	-20.57	-7.44	-7.17	-5.64	-1.63	-20.57	-14.61	-5.64
22	$PPh_2(NMe_2)$	-24.86	-7.33	-6.90	-5.01	-1.63	-24.86	-14.23	-5.01
23	$PPh_2(OEt)$	-23.82	-8.31	-7.57	-5.72	-0.97	-23.82	-15.88	-5.72
24	$P(^tBu)_3$	-23.49	-5.56	-5.54	-3.93	-2.68	-23.49	-11.11	-3.93
25	$PPPh_2Bn$	-23.33	-7.03	-6.09	-5.41	-1.31	-23.33	-13.12	-5.41
26	$PPhBn_2$	-23.24	-7.20	-6.58	-5.19	-1.66	-23.24	-13.77	-5.19
27	$P(OEt)_3$	-24.09	-9.07	-7.83	-5.79	-0.48	-24.09	-16.90	-5.79
28	$P(p\text{-tolyl})_3$	-23.29	-6.67	-6.50	-5.58	-1.38	-23.29	-13.17	-5.58
29	$P(vinyl)_3$	-23.17	-6.68	-6.62	-6.35	-0.94	-23.17	-13.29	-6.35
30	$PPh_2(C_6H_4F)$	-22.45	-6.92	-6.70	-5.57	-1.43	-22.45	-13.62	-5.57
31	$PPh_2(OPh)$	-23.05	-9.19	-7.84	-5.89	-1.39	-23.05	-17.03	-5.89
32	$PPh_2(vinyl)$	-22.81	-6.75	-6.80	-5.86	-1.23	-22.81	-13.55	-5.86
33	$P(C_6H_4Cl)_3$	-21.79	-7.15	-7.02	-5.66	-1.44	-21.79	-14.17	-5.66
34	$P(C_6H_4F)_3$	-21.95	-6.97	-6.78	-5.48	-1.48	-21.95	-13.75	-5.48
35	$PPh(OPh)_2$	-22.31	-9.92	-8.62	-5.71	-1.29	-22.31	-18.55	-5.71
36	$P(benzyl)_3$	-22.69	-6.96	-6.79	-5.12	-1.39	-22.69	-13.75	-5.12
37	$P(^tBu)_2F$	-23.46	-8.68	-7.31	-4.82	-1.55	-23.46	-15.99	-4.82
38	$P(^tBu)F_2$	-21.75	-12.78	-11.39	-6.84	-1.13	-21.75	-24.17	-6.84
39	$P(^nBu)_3$	-25.79	-6.20	-5.91	-5.01	-0.78	-25.79	-12.11	-5.01
40	$P(anis)_3$	-23.50	-6.54	-6.24	-5.38	-1.44	-23.50	-12.78	-5.38
41	$PPh_2(anis)$	-23.01	-6.83	-6.45	-5.58	-1.39	-23.01	-13.28	-5.58

$E_\sigma^d = \Delta E_1$; $E_\pi^{bd} = \Delta E_2 + \Delta E_3$; $E_\sigma^{bd} = \Delta E_4$

ΔE_{rest} = sum of the *intra*fragment polarizations due to minor internal rearrangements (each < 2 kcal/mol).

#5 Figure S1: Plot of calculated *vs.* experimental A_1 *v*(CO)



#6 Table T3: System of linear equations written in matrix form

#	Phosphine	T^{phos}	Ph	Cl	Me	CF_3	C_6F_5	OMe	OPh	Et	F	H	NMe_2	OEt	^{t}Bu	Bn	vinyl	C_6H_4F	tolyl	C_6H_4Cl	^{n}Bu	pOMe
1	$P(C_6F_5)_3$	8.93270	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	$P(OMe)_3$	0.05268	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	$P(OMe)Ph_2$	-3.85386	2	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	$P(OPh)_3$	7.77295	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
5	PCl_2Ph	13.83888	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	PCl_3	26.78391	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	$PClPh_2$	3.76095	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	PEt_3	-16.00158	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
9	PF_3	35.07606	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0
10	PH_2Ph	-1.35648	1	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0
11	$PHPh_2$	-3.75052	2	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
12	PMe_2CF_3	1.31599	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	PMe_2Ph	-11.89375	1	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	PMe_3	-13.56293	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	$PMePh_2$	-8.56776	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	$P(NMe_2)_3$	-12.71490	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0
17	PPh_3	-6.96256	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	PEt_2Ph	-11.88527	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
19	$PEtPh_2$	-9.39799	2	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
20	$PPh(OEt)_2$	-3.99757	1	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
21	$PPh_2(C_6F_5)$	-0.93788	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	$PPh_2(NMe_2)$	-10.41079	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
23	$PPh_2(OEt)$	-4.35471	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
24	$P(^{t}Bu)_3$	-15.43156	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0
25	$PPPh_2Bn$	-8.96325	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
26	$PPhBn_2$	-8.00195	1	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0
27	$P(OEt)_3$	-2.88284	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0
28	$P(p\text{-tolyl})_3$	-8.51212	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
29	$P(vinyl)_3$	-6.73171	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0
30	$PPh_2(C_6H4_F)$	-6.22044	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
31	$PPh_2(OPh)$	-0.60728	2	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
32	$PPh_2(vinyl)$	-6.49614	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0

33	$P(C_6H_4Cl)_3$	-3.89147	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0
34	$P(C_6H_4F)_3$	-5.24056	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0
35	$PPh(OPh)_2$	3.13827	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
36	$P(Bn)_3$	-7.17892	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0
37	$P(^tBu)_2F$	-5.05777	0	0	0	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0
38	$P(^tBu)F_2$	16.19889	0	0	0	0	0	0	0	0	2	0	0	0	1	0	0	0	0	0	0	0
39	$P(^nBu)_3$	-15.88653	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0
40	$P(anis)_3$	-9.92885	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3
41	$PPh_2(anis)$	-7.80919	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Least Square solutions of the system of linear equations has been obtained with Maxima:

Maxima, a Computer Algebra System. Version 5.38.1 (2016) (`http://maxima.sourceforge.net/`)

#7 Equation and parameters used in the multiple regression analysis

Hyper-plane

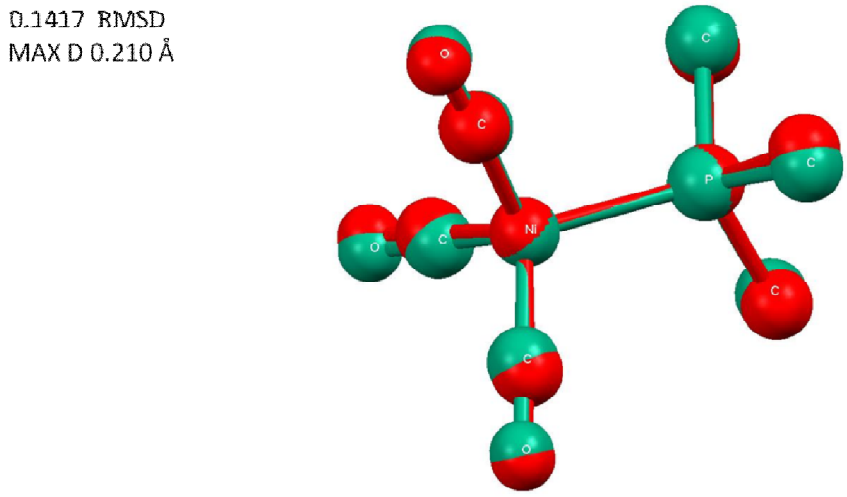
Intercept Value	*Intercept Error*	**S Value**	*S Error*	**P Value**	*P Error*	**B Value**	*B Error*	Statistics Adj. R-Square
2076.58581	*7.00074*	**1.79452**	*0.2007*	**-1.79715**	*0.16771*	**-1.72316**	*0.89628*	0.95929

Data fitting **T^{phos} *vs.* v(CO)**

Intercept Value	Intercept Standard Error	Slope Value	Slope Standard Error	**Statistics Adj. R-Square**
2076.5858	0.34833	1	0.03167	**0.96138**

Intercept: 2076.59 ± 0.35
Slope: 1.00 ± 0.03

#8 Figure S2: comparison between optimized geometry and the structural data of complex $[(CO)_3Ni(P(^tBu)_3)]$ (**24**)

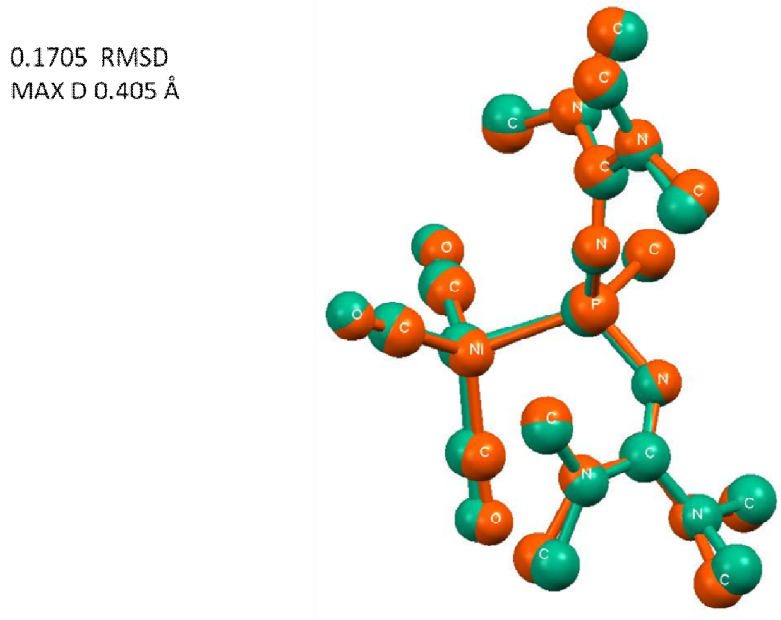


RED: optimized structure (Ni-P 2.320 Å); **GREEN**: structural data from Ref. 50 (Ni-P 2.291 Å)

[Ref. 50 (in the text): Von J. Pickardt, L. Rösch and H. Schumann, *Z. Anorg. Allg. Chem.* 1976, **426**, 66-76].

Note: in the original paper (Ref. 50), only the quaternary carbons of ^tBu groups were reported.

#9 Figure S3: comparison between optimized geometry and the structural data of complex $[(CO)_3Ni(P(Me)(TMG)_2)]$ (TMG: tetramethylguanidine)



RED: optimized structure (Ni-P 2.265 Å); **GREEN**: structural data from Ref. 51 (Ni-P 2.243 Å)

[Ref. 51 (in the text): J. Münchenberg, A. K. Fischer, H. Thönnessen, P. G. Jones and R. Schmutzler, *J. Organomet. Chem.* 1997, **529**, 361-374].

Equation and parameters used in the multiple regression analysis for the definition of parameter **S**

$$d(Ni-P)_{opt} = k_0 + \underbrace{a\cdot\theta \; + b\cdot T^{Phos}}_{S}$$

$k_0 = 206.5 \pm 1.4$

$a = 0.114 \pm 0.01$

$b = -0.202 \pm 0.02$

$Adj.R^2 = 0.9236$

$$S = 0.114\cdot\theta \; - 0.202\cdot T^{Phos}$$

$$d(Ni-P)_{opt} = 206.5 + S$$

$$d(Ni-P)_{opt} = k_1 + c\cdot S$$

$k_1 = 206.5 \pm 0.88$

$c = 1.002 \pm 0.053$

$Adj.R^2 = 0.9294$