Supplementary Material (ESI) for Dalton Transactions
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Supplementary Information

A novel linkage-isomeric pair of dinuclear Pd(II) complexes, bearing a bis-bidentate tetraphos ligand; synthesis, characterization and application in the co- and terpolymerization of CO-ethene and propene

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Energy and Enthalpy values as well as Cartesian atom coordinates for $1a_{5'}$, $1a_{6'}$, 1b', 1c', $2a_{5'}$, $2a_{6'}$, 2b', 2c', $3a_{5'}$, $3a_{6'}$, 3b' and 3c'.

$1a_{5'}$

Energy =-3621.827158 Hartree
Zero-point vibrational energy 407158.9 (Joules/Mol)
Zero-point correction= 0.155079 (Hartree/Particle)
Thermal correction to Energy= 0.176205
Thermal correction to Enthalpy= 0.177149
Thermal correction to Gibbs Free Energy= 0.102881
Sum of electronic and zero-point Energies= -3621.672079
Sum of electronic and thermal Energies= -3621.650953
Sum of electronic and thermal Enthalpies= -3621.650009
Sum of electronic and thermal Free Energies= -3621.724277

1 Pd	0.000000	0.000000	-3.894473
2 Cl	0.574600	-1.659419	-5.450122
3 P	0.489695	-1.567423	-2.283347
4 C	-0.188915	-0.757979	-0.756622
5 H	-0.060584	-2.860913	-2.339611
6 H	1.838880	-1.853547	-1.987425
7 H	-1.279908	-0.846767	-0.852658
8 Pd	0.000000	0.000000	3.894473
9 Cl	0.574600	1.659419	5.450122
10 P	0.489695	1.567423	2.283347
11 C	-0.188915	0.757979	0.756622
12 H	-0.060584	2.860913	2.339611
13 H	1.838880	1.853547	1.987425
14 H	-1.279908	0.846767	0.852658
15 Cl	-0.574600	1.659419	-5.450122
16 P	-0.489695	1.567423	-2.283347
17 C	0.188915	0.757979	-0.756622
18 H	0.060584	2.860913	-2.339611
19 H	-1.838880	1.853547	-1.987425
20 H	1.279908	0.846767	-0.852658
21 Cl	-0.574600	-1.659419	5.450122
22 P	-0.489695	-1.567423	2.283347
23 C	0.188915	-0.757979	0.756622
24 H	0.060584	-2.860913	2.339611
25 H	-1.838880	-1.853547	1.987425
26 H	1.279908	-0.846767	0.852658

$1a_{6'}$

Energy: HF=-3621.8649438
Zero-point vibrational energy 409932.4 (Joules/Mol)

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Zero-point correction= 0.156135 (Hartree/Particle)
Thermal correction to Energy= 0.176755
Thermal correction to Enthalpy= 0.177699
Thermal correction to Gibbs Free Energy= 0.103908
Sum of electronic and zero-point Energies= -3621.708809
Sum of electronic and thermal Energies= -3621.688189
Sum of electronic and thermal Enthalpies= -3621.687245
Sum of electronic and thermal Free Energies= -3621.761035

1	Pd	-0.041508	0.440181	-2.694592
2	Pd	-0.127370	0.345389	4.123688
3	Cl	-1.805678	0.452151	-4.256995
4	Cl	1.762189	0.469930	-4.210901
5	Cl	-0.136194	-1.460043	5.638206
6	Cl	-0.154124	2.107761	5.687914
7	P	-1.744748	0.411279	-1.200892
8	P	1.622708	0.428242	-1.157278
9	P	-0.101529	-1.317094	2.584675
10	P	-0.118361	2.050314	2.631653
11	C	-1.178269	0.389381	0.578392
12	H	-2.046434	0.375559	1.246981
13	C	1.010654	0.400278	0.606749
14	H	1.861320	0.394974	1.297572
15	C	-0.081297	-0.703030	0.821237
16	H	-0.068055	-1.552911	0.129554
17	C	-0.092600	1.485856	0.851784
18	H	-0.088254	2.354777	0.184053
19	H	-2.630931	-0.681312	-1.258035
20	H	-2.641542	1.496359	-1.227844
21	H	2.521486	-0.654979	-1.191454
22	H	2.508461	1.522680	-1.161069
23	H	0.990053	-2.205761	2.616821
24	H	-1.187656	-2.213034	2.588685
25	H	-1.212976	2.935383	2.660773
26	H	0.964718	2.948115	2.688407

1b'

Energy =-1812.1559805
Zero-point vibrational energy 258847.1 (Joules/Mol)
Zero-point correction= 0.098590 (Hartree/Particle)
Thermal correction to Energy= 0.109462
Thermal correction to Enthalpy= 0.110406
Thermal correction to Gibbs Free Energy= 0.060868
Sum of electronic and zero-point Energies= -1812.057391
Sum of electronic and thermal Energies= -1812.046519
Sum of electronic and thermal Enthalpies= -1812.045575
Sum of electronic and thermal Free Energies= -1812.095113

1	Pd	0.000000	0.000000	-3.974346

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2	Cl	0.498714	-1.701903	-5.524683
3	P	0.429413	-1.505568	-2.336529
4	C	-0.116038	-0.761520	-0.704852
5	H	-0.173825	-2.776531	-2.358316
6	H	1.777795	-1.863943	-2.130056
7	H	-1.185217	-0.982891	-0.613437
8	Cl	-0.498714	1.701903	-5.524683
9	P	-0.429413	1.505568	-2.336529
10	C	0.116038	0.761520	-0.704852
11	H	0.173825	2.776531	-2.358316
12	H	-1.777795	1.863943	-2.130056
13	H	1.185217	0.982891	-0.613437
14	H	0.390480	-1.238410	0.139268
15	H	-0.390480	1.238410	0.139268

1c'

Energy =-1851.4787957
Zero-point vibrational energy 335566.7 (Joules/Mol)
Zero-point correction= 0.127811 (Hartree/Particle)
Thermal correction to Energy= 0.139818
Thermal correction to Enthalpy= 0.140762
Thermal correction to Gibbs Free Energy= 0.088099
Sum of electronic and zero-point Energies= -1851.350985
Sum of electronic and thermal Energies= -1851.338978
Sum of electronic and thermal Enthalpies= -1851.338034
Sum of electronic and thermal Free Energies= -1851.390697

1	Pd	-0.003596	0.547670	-2.717853
2	Cl	-1.775376	0.718945	-4.272330
3	Cl	1.763868	0.652478	-4.282993
4	P	-1.702819	0.380351	-1.224111
5	P	1.696957	0.316386	-1.234267
6	H	-0.009875	-0.534473	2.051908
7	C	-1.297006	0.369972	0.592262
8	H	-2.152213	-0.054380	1.127879
9	C	1.301952	0.320574	0.584544
10	H	2.143596	-0.136321	1.114841
11	C	-0.010509	-0.396405	0.964881
12	H	-0.030990	-1.407290	0.536489
13	H	-1.210272	1.415938	0.909101
14	H	-2.468396	-0.791105	-1.384468
15	H	-2.704576	1.362963	-1.315041
16	H	2.417315	-0.882765	-1.399353
17	H	2.734210	1.260892	-1.330990
18	H	1.257035	1.368922	0.902162

2a$_5$'

Energy =-3604.786358 Hartree
Zero-point vibrational energy 410247.3 (Joules/Mol)
Zero-point correction= 0.156255 (Hartree/Particle)
Thermal correction to Energy= 0.176976
Thermal correction to Enthalpy= 0.177920
Thermal correction to Gibbs Free Energy= 0.103912
Sum of electronic and zero-point Energies= -3604.630103
Sum of electronic and thermal Energies= -3604.609382
Sum of electronic and thermal Enthalpies= -3604.608438
Sum of electronic and thermal Free Energies= -3604.682446

1	Pt	0.000000	0.000000	-3.883324
2	Cl	0.548358	-1.649198	-5.493766
3	P	0.476229	-1.556778	-2.288486
4	C	-0.192497	-0.757775	-0.754915
5	H	-0.089089	-2.843076	-2.367786
6	H	1.823754	-1.862409	-2.002002
7	H	-1.283837	-0.841532	-0.847346
8	Pt	0.000000	0.000000	3.883324
9	Cl	0.548358	1.649198	5.493766
10	P	0.476229	1.556778	2.288486
11	C	-0.192497	0.757775	0.754915
12	H	-0.089089	2.843076	2.367786
13	H	1.823754	1.862409	2.002002
14	H	-1.283837	0.841532	0.847346
15	Cl	-0.548358	1.649198	-5.493766
16	P	-0.476229	1.556778	-2.288486
17	C	0.192497	0.757775	-0.754915
18	H	0.089089	2.843076	-2.367786
19	H	-1.823754	1.862409	-2.002002
20	H	1.283837	0.841532	-0.847346
21	Cl	-0.548358	-1.649198	5.493766
22	P	-0.476229	-1.556778	2.288486
23	C	0.192497	-0.757775	0.754915
24	H	0.089089	-2.843076	2.367786
25	H	-1.823754	-1.862409	2.002002
26	H	1.283837	-0.841532	0.847346

$2a_6$'

Energy =-3604.8250731 Hartree
Zero-point vibrational energy 412444.2 (Joules/Mol)
Zero-point correction= 0.157092 (Hartree/Particle)
Thermal correction to Energy= 0.177422
Thermal correction to Enthalpy= 0.178366
Thermal correction to Gibbs Free Energy= 0.104328
Sum of electronic and zero-point Energies= -3604.667981
Sum of electronic and thermal Energies= -3604.647651
Sum of electronic and thermal Enthalpies= -3604.646707
Sum of electronic and thermal Free Energies= -3604.720745

1	Pt	-0.042310	0.444287	-2.684240
2	Pt	-0.126940	0.347685	4.113473
3	Cl	-1.774725	0.471562	-4.314451
4	Cl	1.729236	0.483096	-4.271185
5	Cl	-0.137900	-1.424564	5.700189
6	Cl	-0.157346	2.079667	5.744181
7	P	-1.738325	0.407616	-1.200420
8	P	1.615730	0.423999	-1.158037
9	P	-0.099528	-1.309739	2.586737
10	P	-0.118350	2.044271	2.629797
11	C	-1.177506	0.387407	0.576604
12	H	-2.048658	0.374035	1.240835
13	C	1.010244	0.399460	0.604228
14	H	1.864365	0.395899	1.290379
15	C	-0.080654	-0.703640	0.824633
16	H	-0.067127	-1.557635	0.138395
17	C	-0.092901	1.484144	0.852592
18	H	-0.089503	2.355487	0.188491
19	H	-2.622134	-0.687913	-1.261216
20	H	-2.640548	1.489216	-1.230622
21	H	2.510156	-0.664071	-1.194281
22	H	2.509369	1.513053	-1.167321
23	H	0.991990	-2.199813	2.622731
24	H	-1.185162	-2.207670	2.595742
25	H	-1.212315	2.931400	2.662140
26	H	0.964905	2.943204	2.688707

2b'

Energy =-1803.6366758
Zero-point vibrational energy 260423.9 (Joules/Mol)
Zero-point correction= 0.099190 (Hartree/Particle)
Thermal correction to Energy= 0.109839
Thermal correction to Enthalpy= 0.110783
Thermal correction to Gibbs Free Energy= 0.061375
Sum of electronic and zero-point Energies= -1803.537486
Sum of electronic and thermal Energies= -1803.526837
Sum of electronic and thermal Enthalpies= -1803.525893
Sum of electronic and thermal Free Energies= -1803.575301

1	Pt	0.000000	0.000000	-3.951539
2	Cl	0.484978	-1.675732	-5.567390
3	P	0.431996	-1.501328	-2.328693
4	C	-0.112666	-0.762435	-0.698589
5	H	-0.180281	-2.768485	-2.361967
6	H	1.778256	-1.870542	-2.123099
7	H	-1.180150	-0.989109	-0.602600
8	Cl	-0.484978	1.675732	-5.567390
9	P	-0.431996	1.501328	-2.328693

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10	C	0.112666	0.762435	-0.698589
11	H	0.180281	2.768485	-2.361967
12	H	-1.778256	1.870542	-2.123099
13	H	1.180150	0.989109	-0.602600
14	H	0.400963	-1.237295	0.142268
15	H	-0.400963	1.237295	0.142268

2c'

Energy =-1842.9590317
Zero-point vibrational energy 336768.2 (Joules/Mol)
Zero-point correction= 0.128268 (Hartree/Particle)
Thermal correction to Energy= 0.140134
Thermal correction to Enthalpy= 0.141078
Thermal correction to Gibbs Free Energy= 0.088134
Sum of electronic and zero-point Energies= -1842.830763
Sum of electronic and thermal Energies= -1842.818898
Sum of electronic and thermal Enthalpies= -1842.817953
Sum of electronic and thermal Free Energies= -1842.870897

1	Pt	0.498594	0.027768	-0.072097
2	Cl	2.154727	-1.687646	-0.164312
3	Cl	2.099069	1.798151	-0.062106
4	P	-0.960955	-1.692170	-0.037469
5	P	-1.014548	1.696185	0.062409
6	H	-4.347834	-0.065796	0.500205
7	C	-2.768256	-1.317148	-0.237291
8	H	-3.331855	-2.188710	0.111230
9	C	-2.809512	1.277030	-0.159234
10	H	-3.399712	2.107689	0.241299
11	C	-3.252311	-0.048290	0.494272
12	H	-2.947623	-0.075167	1.548721
13	H	-2.960353	-1.222290	-1.312399
14	H	-0.923733	-2.446850	1.152951
15	H	-0.741710	-2.702352	-0.991912
16	H	-0.998537	2.380912	1.294808
17	H	-0.828749	2.766536	-0.831598
18	H	-3.000748	1.241194	-1.238086

3a$_5$'

Energy =-3707.8617355 Hartree
Zero-point vibrational energy 408189.8 (Joules/Mol)
Zero-point correction= 0.155471 (Hartree/Particle)
Thermal correction to Energy= 0.176267
Thermal correction to Enthalpy= 0.177211
Thermal correction to Gibbs Free Energy= 0.104775
Sum of electronic and zero-point Energies= -3707.706264
Sum of electronic and thermal Energies= -3707.685469

Sum of electronic and thermal Enthalpies= -3707.684524
Sum of electronic and thermal Free Energies= -3707.756961

1	Ni	0.000000	0.000000	-3.852409
2	Cl	0.610145	-1.559864	-5.277332
3	P	0.465811	-1.520307	-2.317421
4	C	-0.190768	-0.757714	-0.756417
5	H	-0.087795	-2.809224	-2.408634
6	H	1.819848	-1.813702	-2.054524
7	H	-1.283613	-0.840141	-0.845269
8	Ni	0.000000	0.000000	3.852409
9	Cl	0.610145	1.559864	5.277332
10	P	0.465811	1.520307	2.317421
11	C	-0.190768	0.757714	0.756417
12	H	-0.087795	2.809224	2.408634
13	H	1.819848	1.813702	2.054524
14	H	-1.283613	0.840141	0.845269
15	Cl	-0.610145	1.559864	-5.277332
16	P	-0.465811	1.520307	-2.317421
17	C	0.190768	0.757714	-0.756417
18	H	0.087795	2.809224	-2.408634
19	H	-1.819848	1.813702	-2.054524
20	H	1.283613	0.840141	-0.845269
21	Cl	-0.610145	-1.559864	5.277332
22	P	-0.465811	-1.520307	2.317421
23	C	0.190768	-0.757714	0.756417
24	H	0.087795	-2.809224	2.408634
25	H	-1.819848	-1.813702	2.054524
26	H	1.283613	-0.840141	0.845269

3a$_6$'

Energy: =-3707.9029534 Hartree
Zero-point vibrational energy 411469.5 (Joules/Mol)
Zero-point correction= 0.156720 (Hartree/Particle)
Thermal correction to Energy= 0.176859
Thermal correction to Enthalpy= 0.177803
Thermal correction to Gibbs Free Energy= 0.106496
Sum of electronic and zero-point Energies= -3707.746233
Sum of electronic and thermal Energies= -3707.726095
Sum of electronic and thermal Enthalpies= -3707.725150
Sum of electronic and thermal Free Energies= -3707.796457

1	Ni	-0.038636	0.443272	-2.665400
2	Ni	-0.131963	0.343240	4.094487
3	Cl	-1.699266	0.456614	-4.112559
4	Cl	1.661096	0.472122	-4.066063
5	Cl	-0.143577	-1.357836	5.493758
6	Cl	-0.159417	2.002461	5.543038
7	P	-1.676593	0.413163	-1.234208

8	P	1.559185	0.429791	-1.189340
9	P	-0.103149	-1.253156	2.617114
10	P	-0.120417	1.982568	2.664590
11	C	-1.174140	0.389244	0.566676
12	H	-2.060840	0.374892	1.211196
13	C	1.007238	0.400888	0.596883
14	H	1.875819	0.395985	1.265760
15	C	-0.081074	-0.699532	0.831311
16	H	-0.067201	-1.567489	0.161758
17	C	-0.093157	1.481819	0.863283
18	H	-0.089066	2.369122	0.219444
19	H	-2.559177	-0.680393	-1.315599
20	H	-2.570488	1.499446	-1.282761
21	H	2.453752	-0.655589	-1.245373
22	H	2.444097	1.524215	-1.213988
23	H	0.990717	-2.137395	2.672194
24	H	-1.189056	-2.148507	2.641257
25	H	-1.215256	2.865836	2.715561
26	H	0.964630	2.875663	2.745065

3b'

Energy =-1855.1743233
Zero-point vibrational energy 259199.0 (Joules/Mol)
Zero-point correction= 0.098724 (Hartree/Particle)
Thermal correction to Energy= 0.109440
Thermal correction to Enthalpy= 0.110384
Thermal correction to Gibbs Free Energy= 0.061874
Sum of electronic and zero-point Energies= -1855.075600
Sum of electronic and thermal Energies= -1855.064883
Sum of electronic and thermal Enthalpies= -1855.063939
Sum of electronic and thermal Free Energies= -1855.112450

1	Ni	0.000000	0.000000	-3.932968
2	Cl	0.521368	-1.608985	-5.346836
3	P	0.399104	-1.459405	-2.375665
4	C	-0.114249	-0.762283	-0.711655
5	H	-0.215385	-2.723112	-2.428565
6	H	1.747901	-1.832289	-2.200962
7	H	-1.181422	-0.986348	-0.602694
8	Cl	-0.521368	1.608985	-5.346836
9	P	-0.399104	1.459405	-2.375665
10	C	0.114249	0.762283	-0.711655
11	H	0.215385	2.723112	-2.428565
12	H	-1.747901	1.832289	-2.200962
13	H	1.181422	0.986348	-0.602694
14	H	0.408678	-1.248654	0.116989
15	H	-0.408678	1.248654	0.116989

3c'

Energy =-1894.4960286
Zero-point vibrational energy 336272.3 (Joules/Mol)
Zero-point correction= 0.128079 (Hartree/Particle)
Thermal correction to Energy= 0.139863
Thermal correction to Enthalpy= 0.140808
Thermal correction to Gibbs Free Energy= 0.089411
Sum of electronic and zero-point Energies= -1894.367949
Sum of electronic and thermal Energies= -1894.356165
Sum of electronic and thermal Enthalpies= -1894.355221
Sum of electronic and thermal Free Energies= -1894.406618

1	Ni	-0.004194	0.554501	-2.693855
2	Cl	-1.668949	0.678114	-4.138595
3	Cl	1.653955	0.610204	-4.150377
4	P	-1.636690	0.406892	-1.249298
5	P	1.631226	0.341106	-1.260863
6	H	-0.009467	-0.542517	2.053722
7	C	-1.289644	0.365091	0.583431
8	H	-2.158557	-0.069387	1.088045
9	C	1.295724	0.313140	0.574279
10	H	2.150039	-0.155893	1.072845
11	C	-0.010533	-0.404858	0.966496
12	H	-0.032376	-1.415724	0.537187
13	H	-1.211043	1.404529	0.923859
14	H	-2.404358	-0.758697	-1.438269
15	H	-2.631636	1.395823	-1.343591
16	H	2.350233	-0.854277	-1.455008
17	H	2.664269	1.289429	-1.362380
18	H	1.261308	1.354876	0.915034

Full reference of 20a

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XRPD pattern of **1a$_5$** and **2a$_5$**