Supporting Information

for

Bi- and Trimetallic Rare-Earth/Palladium Complexes Ligated by Phosphinoamides

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Experimental Section

General Considerations

All manipulations of air-sensitive materials were performed with the rigorous exclusion of oxygen and moisture in flame-dried Schlenk-type glassware either on a dual manifold Schlenk line, interfaced to a high vacuum (10^{-3} torr) line, or in an argon-filled MBraun glove box. Elemental analyses were carried out with an Elementar vario Micro Cube. Hydrocarbon solvents were predried using an MBraun solvent purification system (SPS-800) and then they were degassed, dried and stored in vacuo over $LiAlH_4$. Tetrahydrofuran was distilled under nitrogen from potassium before storage over $LiAlH_4$. Deuterated solvents were obtained from Euro-Isotop (99.5 atom % D) and were degassed, dried and stored in vacuo over Na/K alloy in resealable flasks. IR spectra were obtained on a Bruker Tensor 37 FTIR spectrometer equipped with a room temperature DLaTGS detector and a diamond ATR (attenuated total reflection) unit; for the mid infrared region a KBr beamsplitter was used and for the far infrared region a silicon beamsplitter was used. Raman spectra were recorded on a Bruker MultiRAM spectrometer. $[Li(THF)_4][(Ph_2PNPh)_4Ln]$ (Ln = Y, Lu)[1] were prepared according to literature procedures. $[Pd_2(C_3H_5)_2Cl_2]$ (ABCR) was used as purchased from commercial sources and used without further purification.

Synthesis of $[(Ph_2PNHPh)Pd\{\mu\text{-}(Ph_2PNPh)\}_3Ln(\mu\text{-}Cl)\ Li(THF)_3]$ (Ln = Y (1a), Lu (1b))

1a

THF (15 mL) was condensed at -78°C onto a mixture of 200 mg (0.134 mmol) $[Li(THF)_4][(Ph_2PNPh)_4Y]$, 26 mg (0.077 mmol) $[Pd_2(C_3H_5)_2Cl_2]$ and 6 mg (0.142 mmol) anhydrous LiCl. After stirring over night at room temperature the solution was filtered and the volatiles were removed under reduced pressure. The oily residue was washed with *n*-pentane and then the resulting

solid was dissolved in THF and *n*-pentane was layered on top of the solution. After one day yellow crystals were obtained. Yield 51 mg (0.031 mmol, 22%).

IR (ATR): *ν* (cm^{-1}) = 3363 (w), 3050 (w), 3020 (w), 2920 (w), 2851 (w), 1589 (m), 1559 (w), 1480 (m), 1435 (m), 1395 (w), 1282 (m), 1231 (m), 1180 (w), 1156 (w), 1124 (m), 1097 (m), 1068 (m), 1028 (m), 997 (w), 932 (m), 896 (m), 784 (m), 743 (s), 724 (m), 691 (vs), 627 (m), 613 (m), 596 (m), 534 (s), 508 (s), 476 (s). $C_{88}H_{93}ClLiO_4N_4P_4PdY$ (1632.32): calc C 64.75; H 5.74; N 3.43; found C 64.94; H 5.63; N 3.34.

1b and 1b'

Same procedure as above.

200 mg (0.127 mmol) $[Li(THF)_4][(Ph_2PNPh)_4Lu]$, 25 mg (0.068 mmol) $[Pd_2(C_3H_5)_2Cl_2]$ and 5.7 mg (0.134 mmol) anhydrous LiCl . Yield 100 mg (0.058 mmol, 45%).

IR (ATR): ν(cm^{-1}) = 3382 (w), 3293 (w), 3048 (w), 2973 (w), 2868 (w), 1699 (w), 1684 (w), 1653 (w), 1596 (m), 1559 (w), 1540 (w), 1522 (w), 1494 (m), 1474 (m), 1432 (m), 1390 (w), 1281 (m), 1228 (m), 1177 (w), 1155 (w), 1093 (w), 1067 (w), 1027 (w), 996 (w), 891 (m), 785 (w), 739 (s), 691 (vs), 617 (m), 592 (m), 504 (s).

1b $C_{88}H_{93}ClLiLuO_4N_4P_4Pd$ (1718.38): calc C 61.51; H 5.46; N 3.26; exp C 62.00; H 5.47; N 3.09.

1b' $C_{92}H_{101}ClLiLuN_4O_5P_4Pd$ (1790.49): calc C 61.71; H 5.69; N 3.13; found C 61.66; H 5.21; N 3.31.

$[Li(THF)_4][\{Ph_2PNHPh)Pd\}_2\{\mu$-$(Ph_2PNPh)\}_4Ln]$ (Ln= Y(2a), Lu(2b)

2a

IR (ATR): *ν* (cm^{-1}) = 3365 (w), 3047 (w), 3017 (w), 2973 (w), 2955 (w), 2923 (w), 2872 (w), 2852 (w), 1598 (w), 1586 (m), 1476 (m), 1432 (m), 1395 (w), 1283 (m), 1243 (m), 1179 (w), 1153 (w),

1125 (w), 1089 (w), 1068 (w), 1028 (m), 996 (w), 933 (m), 896 (m), 777 (m), 741 (s), 691 (vs), 627 (m), 611 (m), 595 (m), 506 (s), 482 (s), 454 (s).

2b

IR (ATR): *v* (cm^{-1}) = 3381 (w), 3046 (w), 2974 (w), 2871 (w), 1598 (m), 1494 (m), 1474 (m), 1432 (m), 1392 (w), 1281 (m), 1228 (m), 1180 (w), 1155 (w), 1092 (w), 1067 (w), 1028 (w), 996 (w), 932(m), 895 (m), 780 (w), 740 (s), 691 (vs), 617 (w), 592 (m), 505 (s), 475 (m), 455 (m), 428 (w).

RAMAN: *v* (cm^{-1}) = 3052 (m), 2884 (w), 1584 (s), 1244 (w), 1156 (w), 1090 (m), 1029 (m), 999 (s).

$C_{124}H_{124}LiLuO_4N_6P_6Pd_2$ (2342,94) (**2b**): calcd C 63,57; H 5.33; N 3.59; found C 63.84; H 5.28; N 3.31.

X-Ray-Crystallographic Studies of [Li(THF)$_4$][(Ph$_2$PNPh)$_4$Y], 1a, 1b, 1b', 2a, and 2b. A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fiber. The crystal was transferred directly to the cold stream of a STOE IPDS 2 or STOE StadiVari diffractometer.

All structures were solved by the Patterson method (SHELXS-2013)[2]. The remaining non-hydrogen atoms were located from difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F, minimizing the function $(F_o\text{-}F_c)^2$, where the weight is defined as $4F_0^2/2(F_o^2)$ and F_o and F_c are the observed and calculated structure factor amplitudes using the program SHELXL-2013.[2] Carbon-bound hydrogen atom positions were calculated. The locations of the largest peaks in the final difference Fourier map calculation as well as the magnitude of the residual electron densities in each case were of no chemical significance. Positional parameters, hydrogen atom parameters, thermal parameters, bond lengths and angles have been deposited as supporting information.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary-publication no. CCDC 1400333-1400339. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table S1: Crystal data and structure refinement for **$[Li(THF)_4][(Ph_2PNPh)_4Y]$, 1a, 1b, 1b', 2a, and 2b.**

Compound reference	**$[Li(THF)_4][(Ph_2PNPh)_4Y]$1a**	**1b**	**1b'**	**1b1b`**	**2a**	**2b**
Chemical formula	$C_{72}H_{60}N_4P_4Y$•$C_{16}H_{32}LiO_4$ •3(C_4H_8O)	$C_{88}H_{93}ClLiN_4O_4P_4PdY$ •2(C_4H_8O)	$C_{88}H_{93}ClLiLuN_4O_4P_4Pd$ •2(C_4H_8O)	$C_{76}H_{69}ClLuN_4OP_4Pd$•$C_{16}H_{32}LiO_4$ •C_4H_8O	$C_{90.4}H_{97.8}ClLiLuN_4O_{4.6}P_4Pd$ •C_4H_8O	$C_{108}H_{92}N_6P_6Pd_2Y$ •$C_{16}H_{32}LiO_4$	$C_{108}H_{92}LuN_6P_6Pd_2$ •$C_{16}H_{32}LiO_4$
Formula Mass	1705.69	1776.45	1862.51	1862.51	1833.66	2256.75	2342.81
Crystal system	monoclinic	triclinic	monoclinic	triclinic	triclinic	monoclinic	monoclinic
a/Å	14.911(3)	13.4049(9)	13.559(3)	13.332(3)	13.414(3)	28.427(6)	28.317(6)
b/Å	24.635(5)	15.2317(9)	28.870(6)	15.349(3)	15.386(3)	14.576(3)	14.561(3)
c/Å	26.155(5)	22.790(2)	22.627(5)	21.771(4)	22.048(4)	29.040(6)	29.029(6)
α/°	90	99.348(6)	90	88.53(3)	88.38(3)	90	90
β/°	104.10(3)	98.546(6)	90.84(3)	80.90(3)	80.40(3)	106.14(3)	105.98(3)
γ/°	90	99.455(5)	90	83.96(3)	84.17(3)	90	90
Unit cell volume/Å^3	9318(3)	4455.0(6)	8856(3)	4374.2(16)	4463.2(16)	11559(4)	11507(4)
Temperature/K	200(2)	200(2)	200(2)	150(2)	200(2)	200(2)	200(2)
Space group	$P2_1/c$	P-1	$P2_1/n$	P-1	P-1	$P2_1/c$	$P2_1/c$
No. of formula units per unit cell, Z	4	2	4	2	2	4	4
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
Absorption coefficient, μ/mm^{-1}	0.750	1.007	1.47	1.49	1.456	0.942	1.286
No. of reflections measured	141956	38213	51954	36650	43644	93327	144868
No. of independent reflections	19814	15855	17364	16187	23041	24548	24417
R_{int}	0.1534	0.0719	0.1217	0.0395	0.1767	0.1160	0.0841
Final R_1 values ($I > 2\sigma(I)$)	0.0831	0.0536	0.0579	0.0358	0.0855	0.0752	0.0520
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1728	0.0996	0.0859	0.0933	0.1100	0.1540	0.1509
Final R_1 values (all data)	0.1522	0.1024	0.1967	0.0422	0.2260	0.1614	0.0682
Final $wR(F^2)$ values (all data)	0.2011	0.1122	0.1194	0.0960	0.1476	0.1939	0.1606
Goodness of fit on F^2	1.015	0.892	0.807	1.046	0.831	0.957	1.043

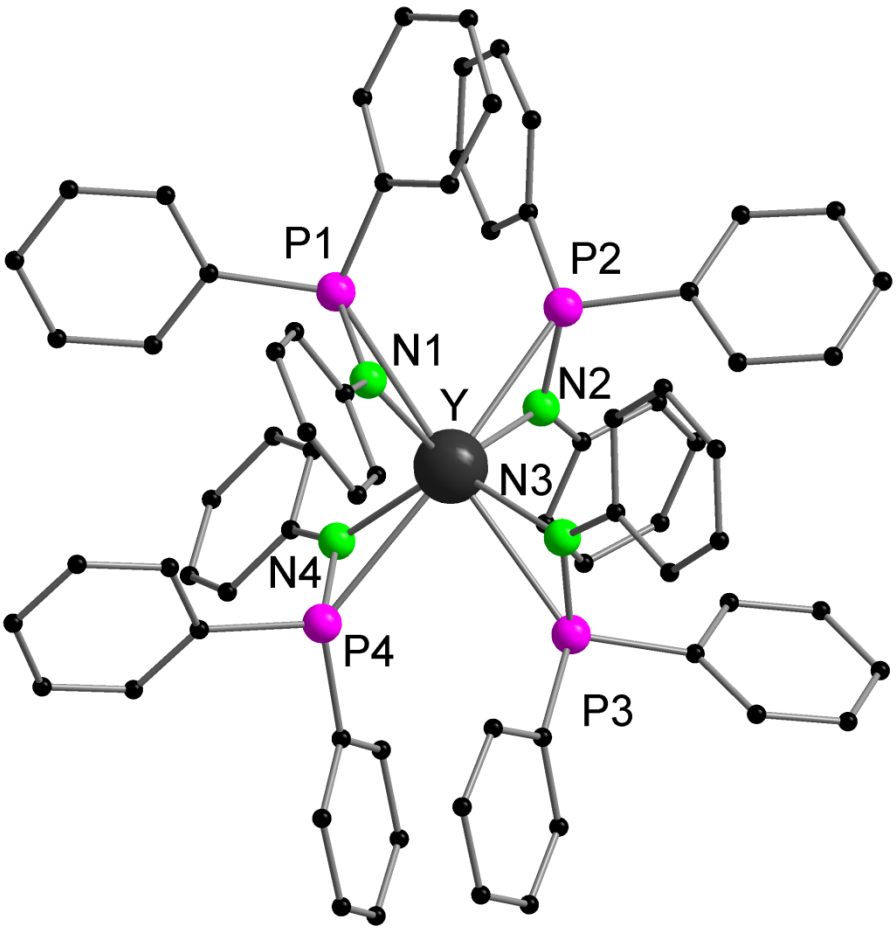

Figure S1: Solid-state structure of the anion of $[Li(THF)_4][(Ph_2PNPh)_4Y]$ (the $[Li(THF)_4]$ cation is disordered). Hydrogen atoms are omitted for clarity. Selected bond lengths [Å], angles [°]: Y-P1 3.0516(14), Y-P2 2.9482(14), Y-P3 2.9957(14), Y-P4 2.9156(15), Y-N1 2.303(4), Y-N3 2.320(4), Y-N2 2.304(4), Y-N4 2.313(4), P1 N1 1.671(4), P2 N2 1.666(4), P3 N3 1.672(4), P4 N4 1.671(4); P1-Y-P2 73.62(4), P1-Y-P3 161.62(4), P1-Y-P4 107.18(4), P2-Y-P3 110.50(4), P2-Y-P4 159.84(4), P3-Y-P4 75.35(4), N1-Y-P1 32.72(9), N1-Y-P2 94.38(10), N1-Y-P3 129.77(10), N1-Y-P4 96.01(10), N1-Y-N2 126.03(14), N1-Y-N3 102.16(14), N1-Y-N4 103.92(14), N2-Y-P1 98.04(10), N2-Y-P2 34.29(10), N2-Y-P3 93.94(11), N2-Y-P4 128.55(10), N2-Y-N3 101.23(14), N2-Y-N4 100.07(14), N3-Y-P1 129.22(10), N3-Y-P2 98.25(10), N3-Y-P3 33.73(10), N3-Y-P4 96.38(10), N4-Y-P1 95.40(10), N4-Y-P2 125.37(10), N4-Y-P3 96.17(10), N4-Y-P4 34.94(10), N4-Y-N3 126.16(14).

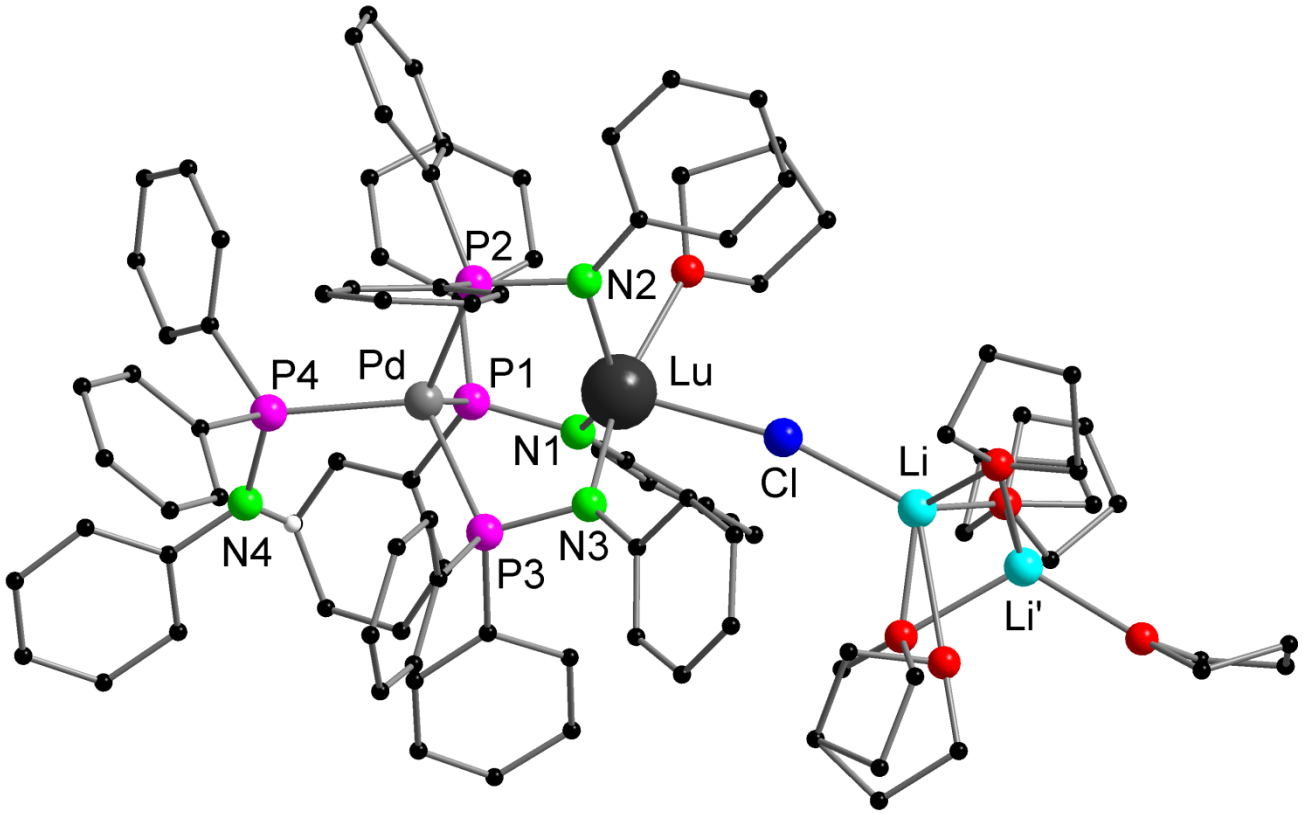

Figure S2: Solid-state structure of co-crystallized **1b** and **1b'** in a 2:3 ratio.

NMR Data of [(Ph_2PNHPh)Pd{μ-(Ph_2PNPh)}$_3$Ln(μ-Cl) Li(THF)$_3$] (Ln = Y (1a), Lu (1b))

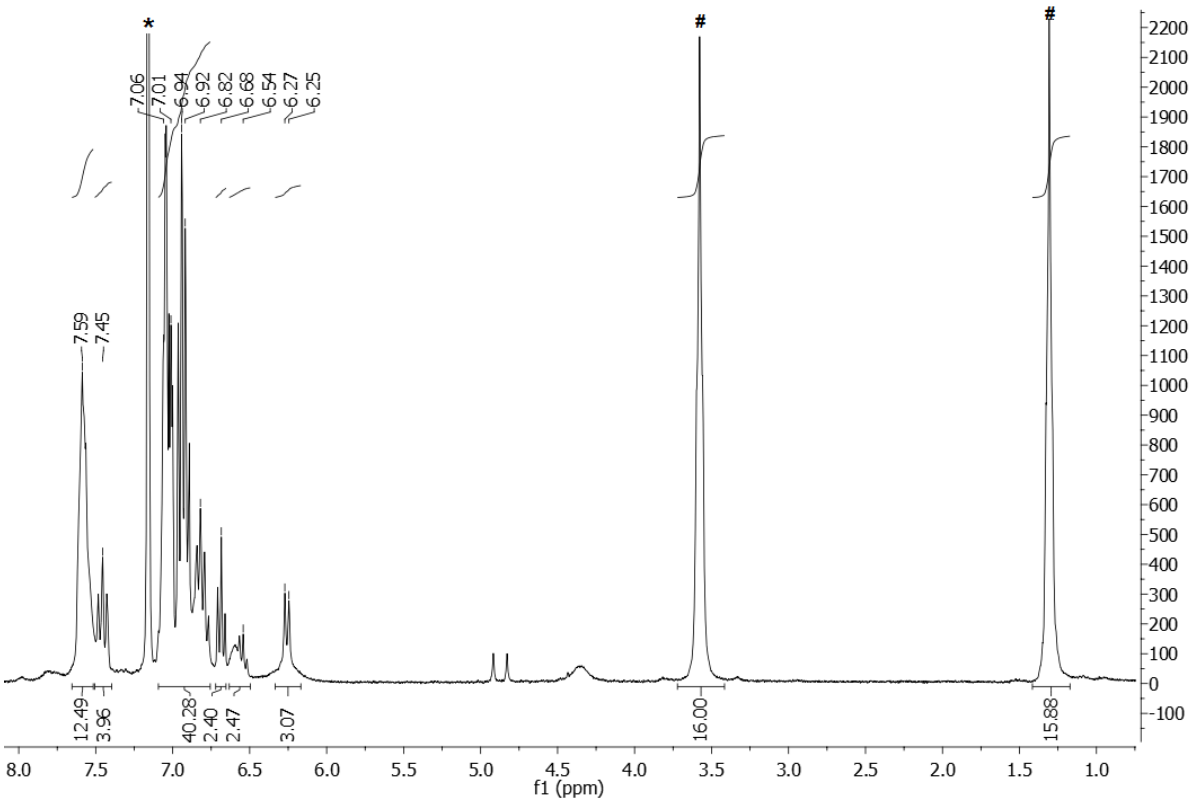

Figure S3: ^{1}H NMR spectrum (C_6D_6, 300MHz) of **1a**. *C_6D_6, #coordinated THF. Due to the fast decomposition of **1a** in solution, the integration values do not perfectly fit the expected values.

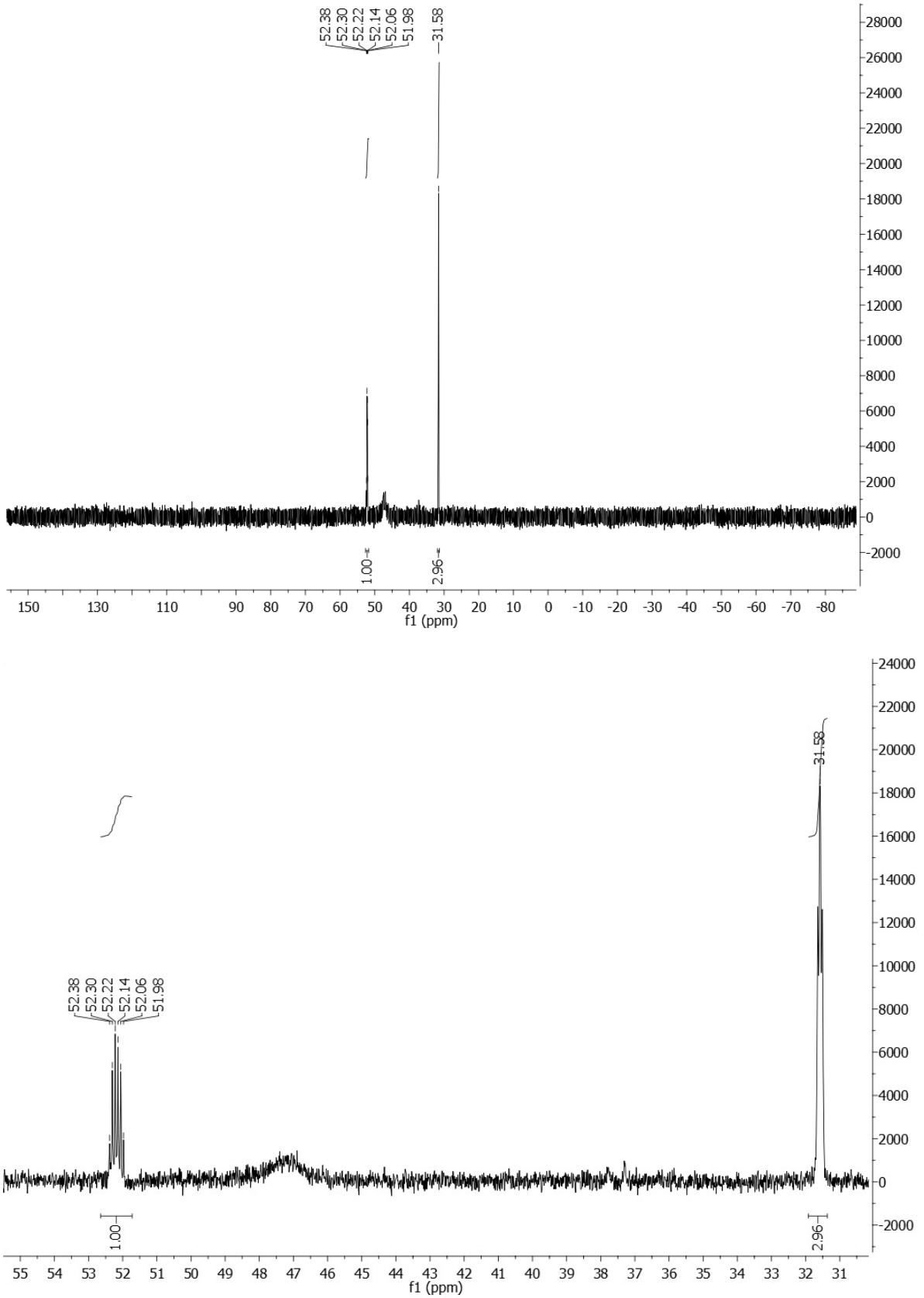

Figure S4: $^{31}P\{^{1}H\}$ NMR spectrum (C_6D_6, 121MHz) of **1a**; full spectrum (top) and detailed spectrum 5 (bottom). Due to the fast decomposition of **1a** in solution, only the main peaks are labeled.

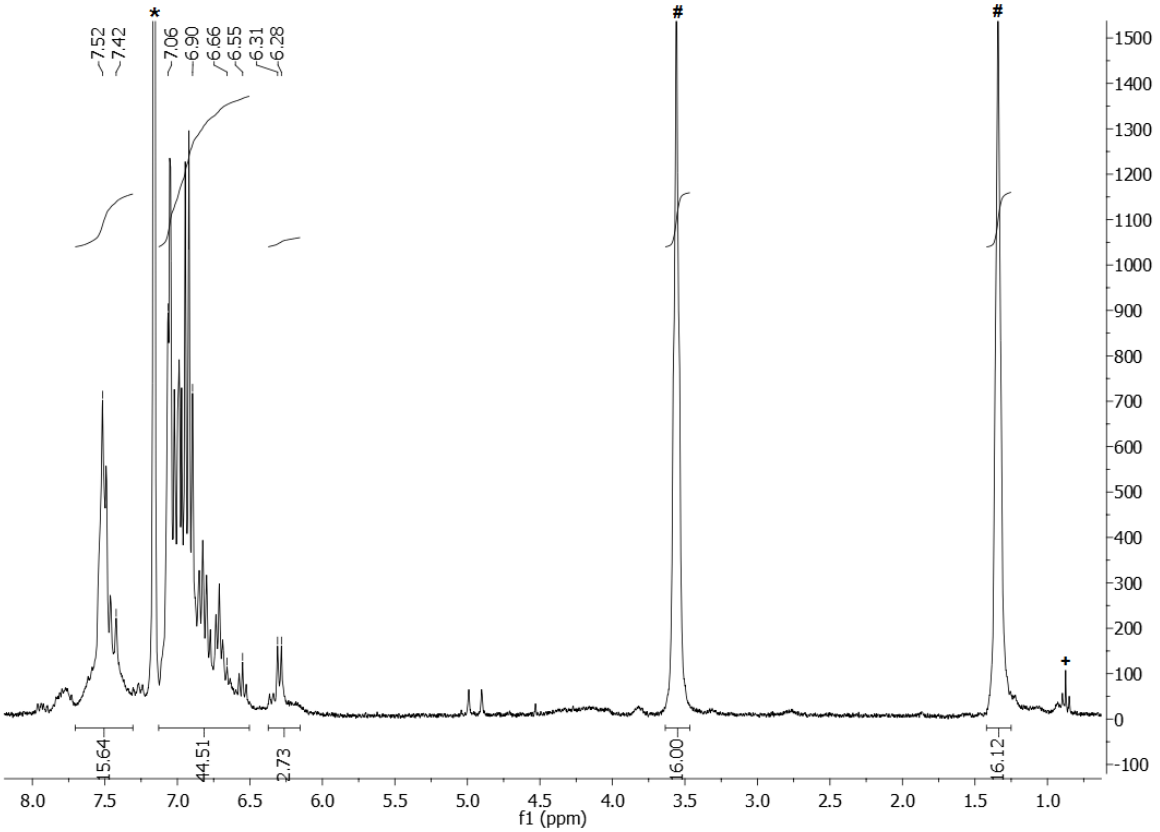

Figure S5: ^{1}H NMR spectrum (C_6D_6, 300MHz) of **1b**. *Solvent peak C_6D_6, $^{\#}$coordinated THF, $^{+}$*n*-pentane. Due to the moderate solubility of **1b** in C_6D_6 and its fast decomposition in solution, the integration values do not perfectly fit the expected values.

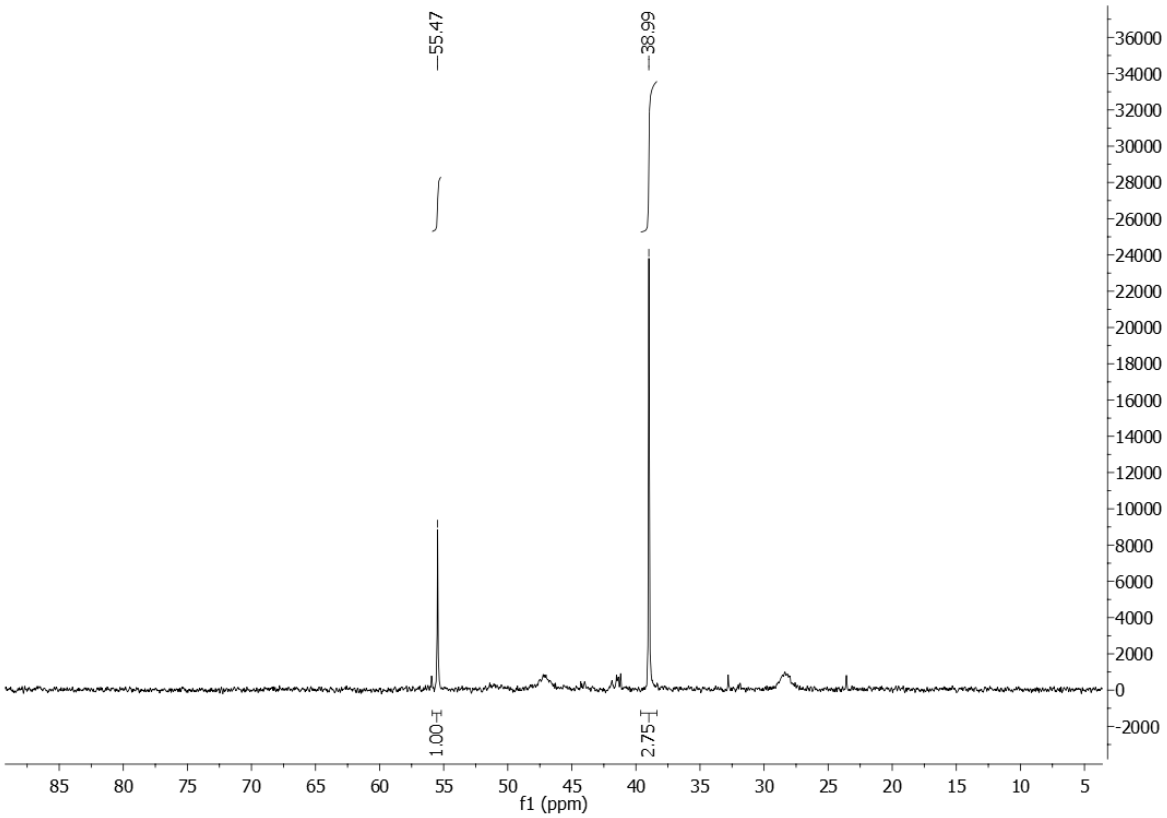

Figure S6: $^{31}P\{^{1}H\}$ NMR spectrum (C_6D_6, 121MHz) of **1b**. Due to the fast decomposition of **1b** in solution only the main peaks are labeled.

Quantum chemical calculations

Table S2: DFT optimized structure parameters of **1b'** (without counter ion): Functional dependence and comparison to experiment for different functionals: BP86[3], TPSSh[4], PBE0, and PBE0-D3

	Experiment	BP86	TPSSh	PBE0	PBE0-D3
Pd-Lu	**2.9712**	3.054	3.007	3.011	**2.985**
Lu-N(1)	2.2602	2.272	2.295	2.292	2.278
Lu-N(2)	2.2705	2.301	2.269	2.264	2.248
Lu-N(3)	2.3139	2.334	2.332	2.382	2.316
Lu-O	2.4412	2.580	2.549	2.556	2.475
Lu-Cl	2.5690	2.536	2.543	2.540	2.533
Pd-P(1)	2.3548	2.387	2.397	2.385	2.342
Pd-P(2)	2.3570	2.399	2.399	2.376	2.319
Pd-P(3)	2.3574	2.402	2.380	2.370	2.333
Pd-P(4)	2.3915	2.448	2.450	2.435	2.384
Lu-Pd-P(2)	175.3	175.1	175.3	174.9	174.1
Pd-Lu-Cl	160.7	161.7	161.6	162.2	162.3
Cl-Lu-N(3)	105.6	105.7	105.0	105.2	105.2
P(2)-Pd-P(4)	110.1	109.9	109.7	109.9	109.2

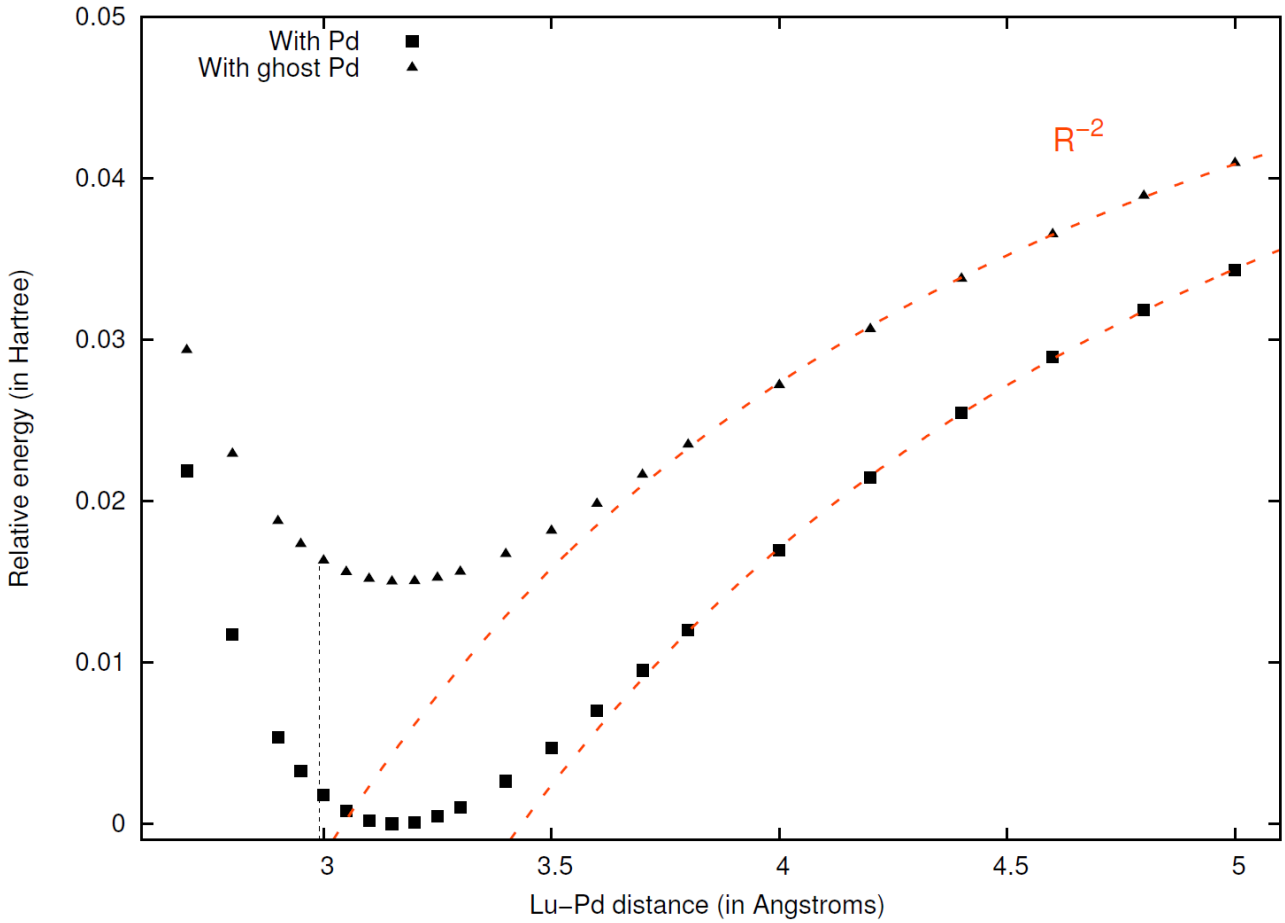

Figure S7: Potential energy curve of model **b**. The long-range behaviour is typical for a charge-dipole interaction.

Optimized structures from the quantum chemical calculations (xyz-file format)
Coordinates of complex 1b, optimized at the PBE0-D3/def2-TZVP level of theory

157
Energy =
C -0.2482000 11.5218820 13.5796667
C 1.1340443 11.5496337 13.6971958
C 1.7722399 12.7634620 13.8996026
C 1.0408638 13.9383810 13.9885734
C -0.3466387 13.9242386 13.8506588
C -0.9788854 12.6968905 13.6458806
P -1.2719872 15.5043083 14.0230971
N -0.3070427 16.7207251 13.4271494
C 0.5394417 16.6337844 12.3295233
C 0.5004699 15.6107985 11.3671338
C 1.3875178 15.5876107 10.3031610
C 2.3451833 16.5783964 10.1477299
C 2.3995950 17.5971171 11.0909752
C 1.5238865 17.6220659 12.1604802
Lu -1.0265981 18.5086053 14.7121775
N 0.2142250 18.5398893 16.5868846
C 0.9053381 19.5722233 17.2184386
C 2.1565237 19.4223003 17.8278084
C 2.7778092 20.4894041 18.4569613
C 2.1774869 21.7388134 18.4965076
C 0.9344964 21.9017735 17.8978243
C 0.3079301 20.8378385 17.2764768

O	-2.3441444	18.9383353	12.6619343
C	-3.7345368	19.1932528	12.4483807
C	-3.7996469	20.4781501	11.6179153
C	-2.3519577	20.6810829	11.1426831
C	-1.6989799	19.3504022	11.4566236
N	-3.0081326	19.1042861	15.6649752
P	-3.4231958	17.7409324	16.5288356
C	-5.1259652	17.2495941	16.0222670
C	-6.2261453	17.1661671	16.8744780
C	-7.4629713	16.7531442	16.3986497
C	-7.6271903	16.4343339	15.0589020
C	-6.5378411	16.5140712	14.2019736
C	-5.2999822	16.9025573	14.6841718
Pd	-1.8233762	16.0587331	16.2206959
P	-2.2856396	14.0359314	17.2558888
C	-3.6792881	13.0643070	16.5872551
C	-4.9331672	13.6741048	16.5164482
C	-5.9973177	13.0378498	15.9002599
C	-5.8183801	11.7877375	15.3218022
C	-4.5716806	11.1817004	15.3702061
C	-3.5089570	11.8119435	16.0024921
P	0.1797144	16.9709378	17.1375990
C	0.4193464	17.0973275	18.9570722
C	1.4508481	16.5024192	19.6798289
C	1.5389599	16.6602266	21.0558833
C	0.6097174	17.4348199	21.7323394
C	-0.4099804	18.0486578	21.0190727
C	-0.5070136	17.8743317	19.6499347
Cl	0.2881904	20.5038630	13.8713435
C	-3.7279404	20.2858487	15.5607479
C	-5.0658665	20.4473523	15.9556802
C	-5.7247913	21.6543747	15.7872349
C	-5.0853334	22.7498335	15.2259206
C	-3.7581525	22.6111197	14.8397121
C	-3.0930408	21.4096316	15.0016470
C	-2.6465918	15.2117985	12.8393092
C	-2.7051396	15.8721791	11.6144034
C	-3.7767233	15.6812682	10.7546175
C	-4.8075614	14.8190040	11.1010260
C	-4.7705504	14.1720148	12.3281716
C	-3.7111854	14.3839590	13.1953357
C	-3.6952814	18.2586425	18.2604153
C	-4.0041557	17.2871402	19.2121909
C	-4.1426146	17.6172234	20.5486566
C	-3.9539134	18.9302063	20.9610513
C	-3.6133456	19.8986025	20.0291009
C	-3.4844919	19.5669744	18.6870205
C	1.7422016	16.1660522	16.6198823
C	2.5716439	16.8000230	15.6983877
C	3.7173160	16.1750479	15.2284710
C	4.0637729	14.9130104	15.6892839
C	3.2383612	14.2665660	16.5999127
C	2.0774595	14.8784648	17.0424802
C	-2.5943759	13.9823199	19.0576220
C	-3.8165788	13.6433754	19.6329928
C	-3.9954833	13.7298375	21.0067174
C	-2.9551103	14.1470007	21.8232517
C	-1.7318095	14.4805697	21.2573658
C	-1.5571823	14.4038649	19.8873033
N	-0.9386786	13.0193161	17.0776718
C	-0.5619730	11.8155527	17.6480955
C	-1.3697650	11.1023538	18.5364860
C	-0.9241610	9.9071295	19.0773383
C	0.3195645	9.3891692	18.7491791
C	1.1200819	10.0911030	17.8570386
C	0.6901933	11.2867115	17.3137662
H	-0.2834066	13.3890490	16.4038604
H	-1.9025588	16.5416388	11.3379147
H	-5.5963102	19.6179534	16.4000173
H	-3.7317656	13.9280150	14.1772949
H	-0.2308480	14.8187421	11.4552666
H	2.3076145	17.7916077	15.3483665

H 2.8508615 12.8072846 13.9922286
H 1.5539856 14.8782212 14.1459872
H 1.5833381 18.4278758 12.8827479
H -4.1040713 16.2520564 18.9075898
H -1.9002928 18.6068419 10.6744389
H -0.6292196 19.4055405 11.6413067
H 1.4236141 14.3466282 17.7260073
H -4.0475260 19.1911658 22.0096197
H 2.6464814 18.4576845 17.8079061
H -3.4365780 20.9209819 20.3442502
H 1.3227732 14.7764570 9.5850542
H -0.7642547 10.5796548 13.4301069
H -3.1999822 20.3270848 17.9721477
H -4.2149288 19.2701235 13.4182649
H -4.1563177 18.3407890 11.9043140
H -2.3450234 11.4830289 18.8046595
H -2.0555489 21.3328979 14.6912004
H 1.3114741 11.8225296 16.6046984
H 1.7070048 10.6310351 13.6386341
H -3.0975274 14.2172472 22.8958870
H 2.0936329 9.7031789 17.5768677
H -5.6057944 23.6918990 15.0988394
H -5.5818296 13.5204007 12.6326014
H -6.9558502 13.5403944 15.8448864
H -5.0671330 14.6776435 16.9042674
H 4.3385044 16.6792965 14.4968657
H -3.2246188 23.4509566 14.4063720
H 2.2116349 15.9257025 19.1707877
H 3.0360386 16.5563130 9.3128212
H -3.8010013 16.2052088 9.8047801
H -4.6336117 13.3014941 19.0089654
H -4.4201548 10.2119966 14.9088085
H -4.4908389 20.3594591 10.7812372
H -4.1412791 21.3159207 12.2251222
H -2.0532170 12.6515549 13.5292341
H 0.6585552 8.4533475 19.1772256
H -5.6419349 14.6648893 10.4254636
H 3.7468025 20.3373691 18.9213395
H -0.6699378 20.9687865 16.8275957
H -4.3677993 16.8393694 21.2690585
H 3.1383486 18.3867179 10.9994216
H -2.2780993 20.9395863 10.0852080
H -1.8583613 21.4594854 11.7266882
H 2.3520137 16.1864575 21.5958153
H 3.4877837 13.2714901 16.9525128
H -1.3053186 18.3599205 19.1061901
H -1.5687593 9.3738335 19.7676082
H -2.5359367 11.3381451 16.0211827
H 2.6669706 22.5713420 18.9891065
H -6.7593349 21.7341341 16.1053819
H 0.4411030 22.8678545 17.9202153
H 4.9645643 14.4285318 15.3290455
H -6.6443027 11.2956849 14.8201331
H -0.9115392 14.8229618 21.8768059
H -0.6075876 14.6911484 19.4544769
H -1.1422350 18.6654283 21.5256449
H 0.6832867 17.5656142 22.8065111
H -6.1230687 17.4389836 17.9177673
H -4.4466132 16.9196660 14.0178116
H -8.3050058 16.6936445 17.0802071
H -6.6411914 16.2520233 13.1556645
H -8.5956908 16.1201123 14.6854822
H -4.9546101 13.4646881 21.4384861

****

Coordinates of model a

37
Energy =
C -1.9817182 19.1715971 11.2716784
O -2.6060703 18.8541727 12.5072956

C	-3.8237661	19.5773426	12.5307732
C	-3.4506760	20.9487921	11.9951137
C	-2.3665347	20.6241603	10.9559550
Lu	-1.0510469	18.5219292	14.5708045
P	-3.4696942	17.4843048	16.2840566
Pd	-1.7773832	15.8952488	16.0559919
P	-2.1234667	13.8813587	17.0703625
N	-0.8159457	13.3485873	18.0490023
P	-1.0188949	15.4867977	13.8891334
N	-0.4373727	16.8709755	13.2036760
H	-1.8779087	14.8577051	12.9269356
N	-3.0105196	18.9072690	15.5721110
Cl	-0.1228392	20.7341402	13.7021462
N	0.3652969	18.3769667	16.2540484
P	0.0038306	17.0159327	17.1111779
H	-3.5460790	19.7325140	15.8058614
H	1.1006966	18.9790356	16.5949678
H	-0.0395882	16.7964779	12.2776010
H	-4.8265078	17.2331556	15.8848808
H	-2.3680581	12.7223912	16.2678375
H	-3.1815122	13.5606660	17.9697294
H	-3.8443954	17.8061939	17.6277469
H	-0.1381199	17.3986502	18.4842793
H	1.2390700	16.3231042	17.3548532
H	-0.0020092	14.4851434	13.7433775
H	-0.6893140	12.3533861	18.1642743
H	0.0408353	13.7905613	17.7484339
H	-2.3493093	18.4811546	10.5011108
H	-0.9097016	19.0305942	11.3958160
H	-4.1839317	19.5559938	13.5575279
H	-4.5534623	19.0784173	11.8746727
H	-4.3050550	21.4826400	11.5734937
H	-3.0219660	21.5473255	12.8003564
H	-2.7413677	20.7140939	9.9335633
H	-1.5074675	21.2837705	11.0730380

****

Coordinates of model b

43

Energy =

C	6.8565741	14.5355959	6.8935331
C	6.8527501	13.4479332	5.8062144
C	5.7158234	12.5367235	6.2306333
O	5.7377924	12.5985885	7.6570978
C	5.9148153	13.9820421	7.9679088
Lu	5.8257854	10.4889971	9.0981334
N	3.8880799	10.3882751	8.0104648
N	6.2538822	8.4629906	9.9785262
Pd	3.9751759	10.3493851	11.4551958
P	2.3650343	10.1600631	13.1923083
N	1.2904426	8.8999015	12.7897494
N	6.9906980	11.9305096	10.3250581
Cl	7.4152079	9.8317602	7.2296940
P	4.0149789	8.0875197	10.6354060
P	5.9249603	10.7287850	12.7022144
P	2.9453202	11.9480766	10.1195062
H	1.4162316	11.1501089	13.5800232
H	0.8120588	8.4017966	13.5252282
H	3.5006640	12.8952904	9.2315344
H	1.8300535	11.6139147	9.3272914
H	2.6974552	9.8529022	14.5499159
H	3.9700959	7.6274069	9.3074374
H	3.2028361	9.6553043	8.1525907
H	6.7575051	8.4106436	10.8574970
H	6.7298381	12.7451164	10.8655979
H	5.7747034	10.3200701	14.0702010
H	6.4673542	11.9881196	13.0485183
H	2.6947932	7.4717459	10.8914579
H	1.7120245	8.2768667	12.1177466
H	4.7473117	12.9105554	5.8718524

H	5.8383144	11.4987388	5.9324333
H	6.3084742	14.0536721	8.9776965
H	4.9352116	14.4731609	7.9289538
H	6.4910972	15.4933456	6.5174752
H	7.8573528	14.6912609	7.2962430
H	6.7062431	13.8464091	4.8006827
H	7.7867438	12.8838734	5.8199244
H	7.9960358	11.9863336	10.1914771
H	7.1677920	10.0794862	12.5361105
H	6.6982051	7.7988408	9.3515394
H	4.6477947	7.0163370	11.2931528
H	3.7085790	10.7728230	7.0904220
H	2.2492134	12.9390634	10.8966569

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