

Supplementary Information for the manuscript:

**Further Orthometalated Dinuclear Palladium(III) Compounds with
Bridging N,S-Donor Ligands**

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80101 Joensuu, Finland

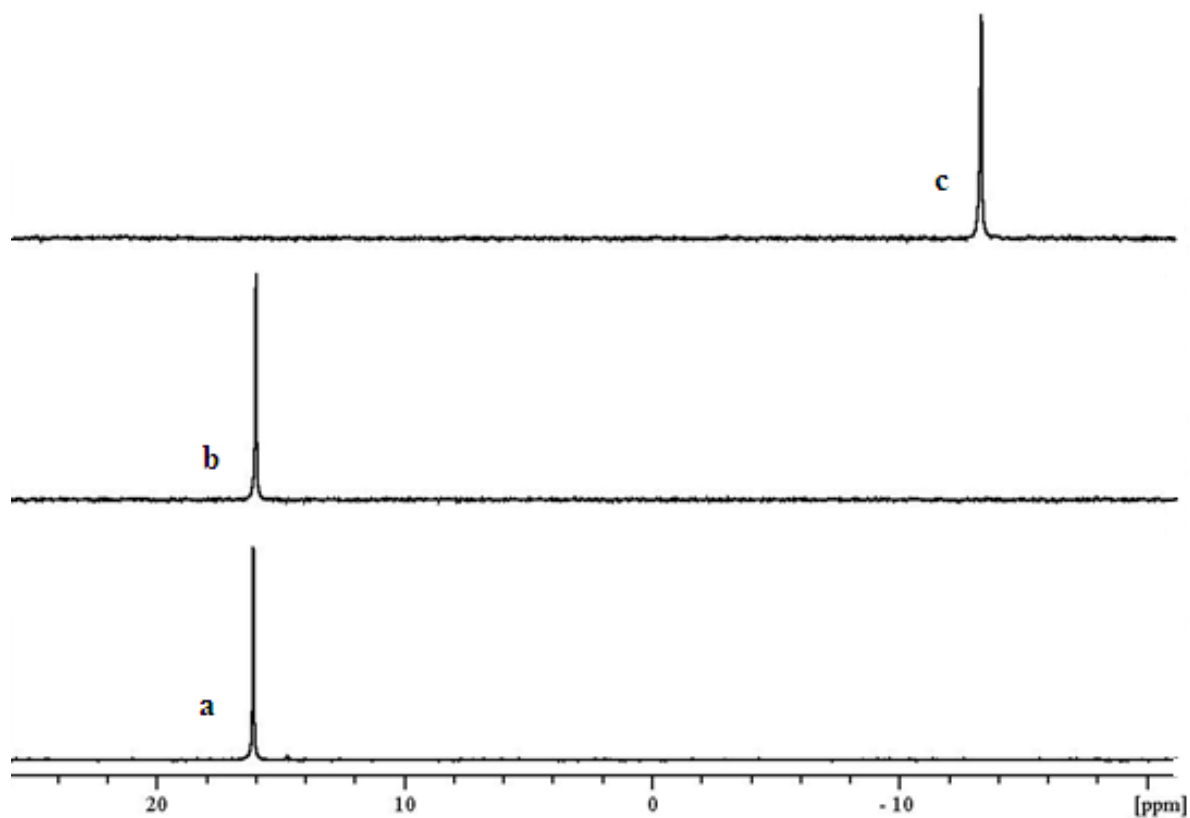


Figure S1. ^{31}P NMR spectra of compound **2g** at 298K (a) and 200K (b). ^{31}P NMR spectrum at 200 K of compound **3g** obtained by addition of PhICl_2 to a solution of compound **2g** in CD_2Cl_2 (c).

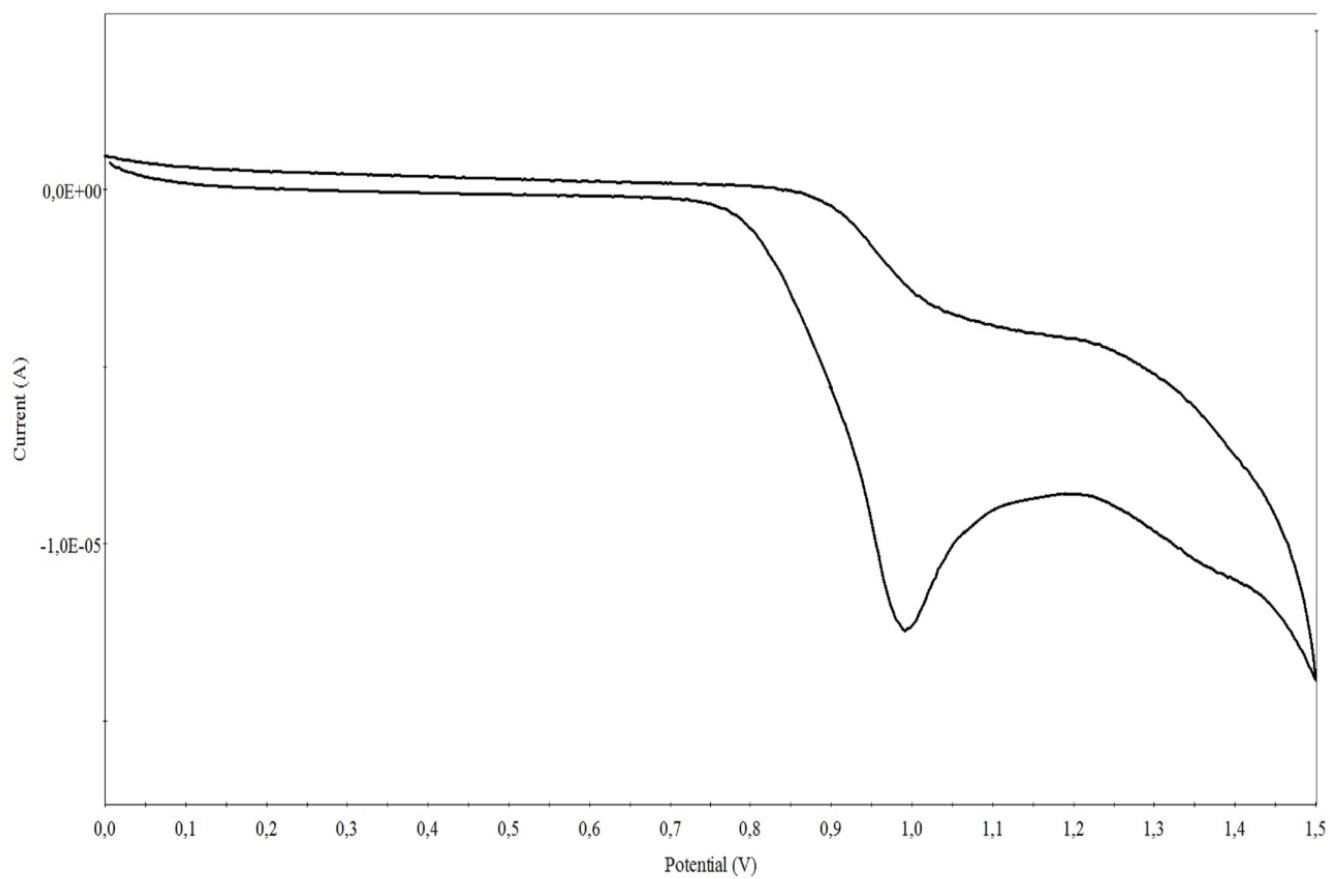


Figure S2. Cyclic voltammogram of compound **2f** in CH_2Cl_2

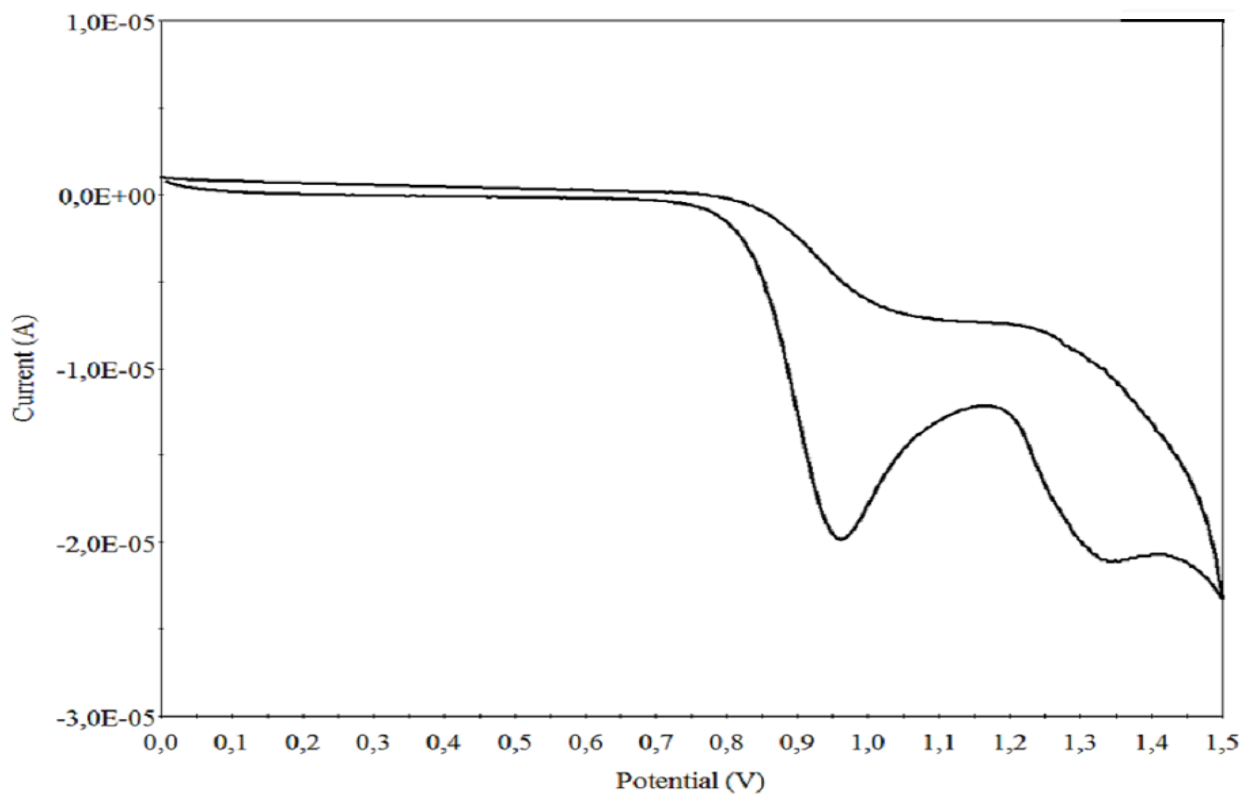


Figure S3. Cyclic voltammogram in CH_2Cl_2
of compound **2f** with the addition of 2 equivalents of TEACl

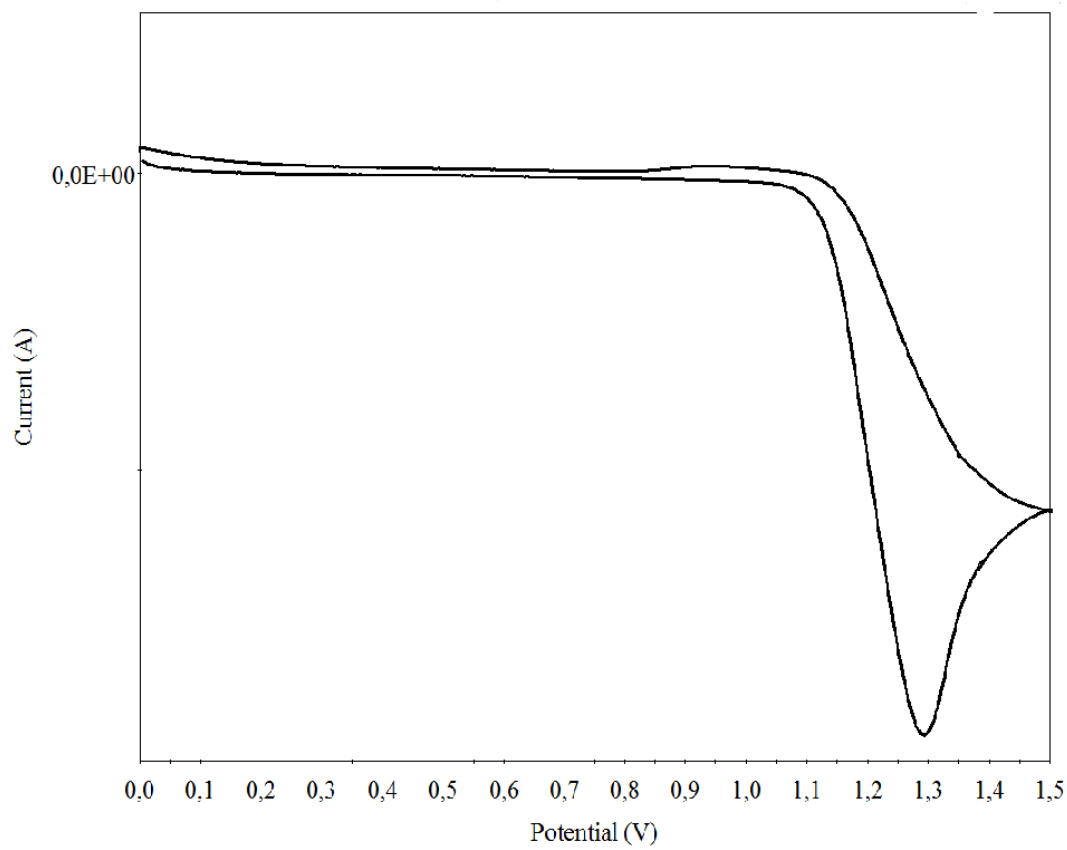


Figure S4. Cyclic voltammogram of TEACl in CH₂Cl₂

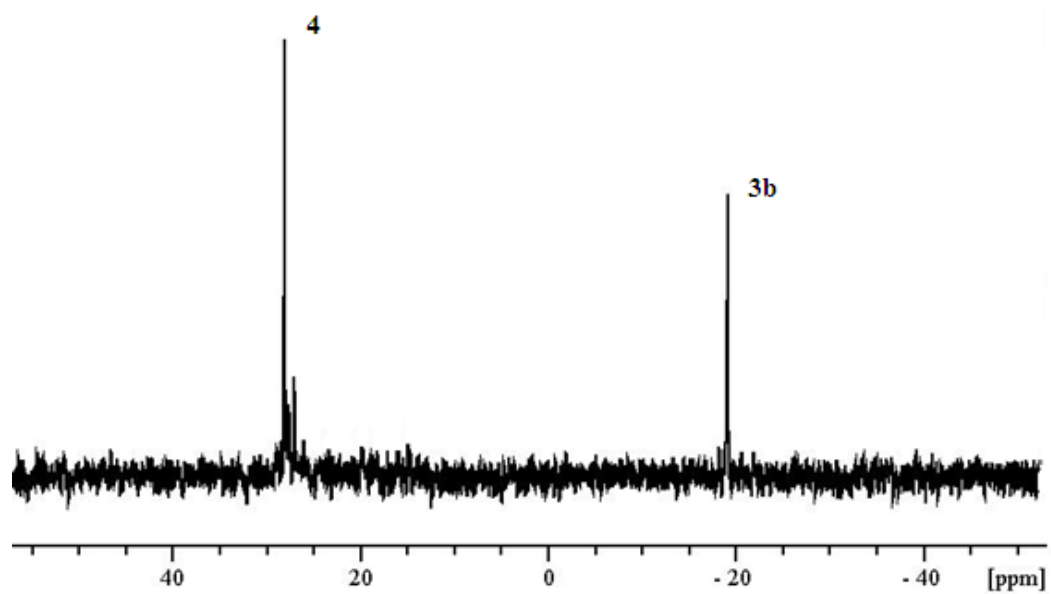
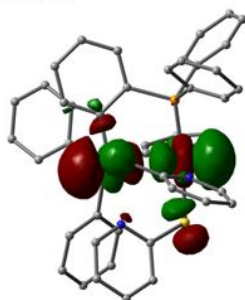
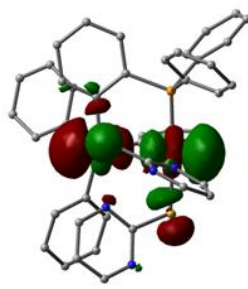


Figure S5. ^{31}P NMR spectrum of the reaction of **2b** with PhICl_2 in CH_2Cl_2 at 200K

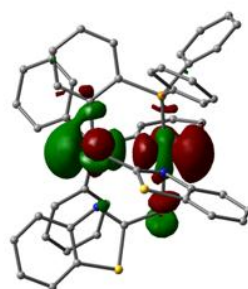
HOMO



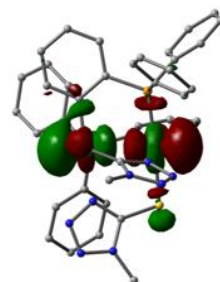
2a



2d

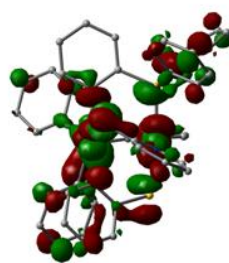


2g

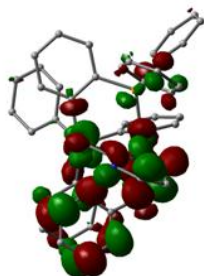


2h

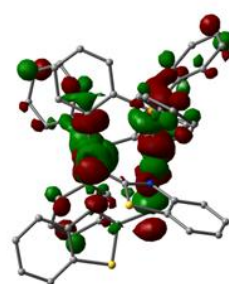
LUMO



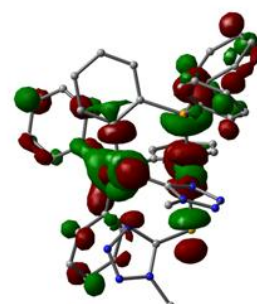
2a



2d



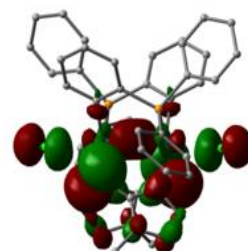
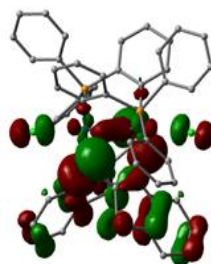
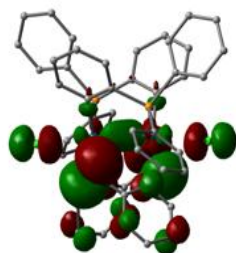
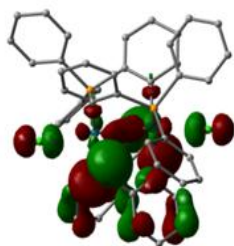
2g



2h

Figure S6. Frontier molecular orbitals for Pd(II) complexes with N,S ligands

HOMO



LUMO

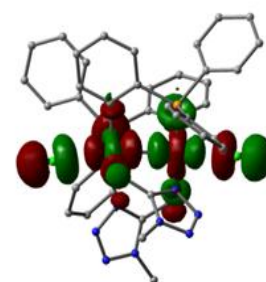
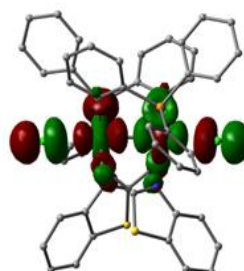
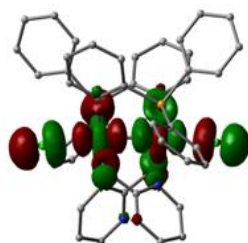
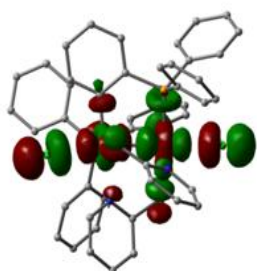


Figure S7. Frontier molecular orbitals for Pd(III) complexes with N,S ligands

Table S1. Properties of the electron density at the Pd-S (Pd-O) and Pd-N bond critical points (BCPs) for complexes Pd₂[(C₆H₄)PPh₂]₂[N-S]₂ and Pd₂[(C₆H₄)PPh₂]₂[N-S]₂Cl₂. The selected properties are ρ(BCP) = local electron density at the BCP; Laplacian = second derivative of ρ; ε = ellipticity, which represents the cylindricity of the charge distribution; |V|/G = ratio of potential energy density and kinetic energy density; |λ₁/λ₃ = ratio between perpendicular and parallel curvatures of the bond paths; E_{int} = interaction energy between two interacting atoms; Ω(Pd,X) = delocalization index between Pd and X atoms (X=S, N or O).

complex	BCP	ρ(BCP) e/Å ³	Laplacian e/Å ⁵	ε	V /G	λ ₁ /λ ₃	E _{int} kJmol ⁻¹	Ω(Pd,X)
Pd₂[(C₆H₄)PPh₂]₂[N-S]₂								
2a	Pd-S	0.5516	4.1844	0.0773	1.33	0.24	-114.2	0.76
	Pd-N	0.5028	8.3264	0.1264	1.08	0.15	-133.4	0.51
2b	Pd-S	0.5433	4.1181	0.0761	1.33	0.23	-111.7	0.74
	Pd-N	0.5026	8.2149	0.1363	1.08	0.15	-132.2	0.51
2c	Pd-S	0.5481	4.1992	0.0774	1.33	0.23	-113.6	0.74
	Pd-N	0.5000	8.1348	0.1368	1.08	0.15	-130.9	0.51
2d	Pd-S	0.5619	4.2140	0.0742	1.34	0.24	-116.7	0.77
	Pd-N	0.4913	8.2486	0.1242	1.08	0.15	-130.5	0.50
2e	Pd-S	0.5278	4.1153	0.0838	1.32	0.23	-108.4	0.73
	Pd-N	0.5458	9.1605	0.1083	1.09	0.15	-150.3	0.55
2f	Pd-S	0.5232	4.1715	0.0840	1.31	0.23	-108.1	0.71
	Pd-N	0.5401	9.0605	0.1131	1.09	0.15	-148.1	0.54
2g	Pd-S	0.5286	4.1807	0.0835	1.32	0.23	-109.4	0.71
	Pd-N	0.5132	8.5901	0.1212	1.08	0.15	-138.1	0.51
2h	Pd-S	0.5143	4.1600	0.0876	1.30	0.23	-106.1	0.70
	Pd-N	0.5397	9.4446	0.1286	1.08	0.15	-152.1	0.52
Pd₂[(C₆H₄)PPh₂]₂[N-S]₂Cl₂								
3a	Pd-S	0.5652	3.6773	0.0639	1.38	0.26	-110.7	0.73
	Pd-N	0.4663	6.9417	0.0789	1.08	0.16	-111.4	0.47
	Pd-Cl	0.4045	3.9378	0.0106	1.19	0.19	-79.5	0.56
3b	Pd-S	0.5746	3.7259	0.0623	1.38	0.26	-113.3	0.74
	Pd-N	0.3748	5.3271	0.0820	1.05	0.15	-80.9	0.41
	Pd-Cl	0.3987	3.8720	0.0112	1.19	0.19	-77.9	0.56
3c	Pd-S	0.5481	4.1992	0.0774	1.33	0.25	-113.6	0.74
	Pd-N	0.5000	8.1348	0.1368	1.08	0.15	-130.9	0.41

	Pd-Cl	0.4032	3.8940	0.0117	1.20	0.19	-78.8	0.57
3d	Pd-S	0.5686	3.6443	0.0612	1.38	0.26	-110.9	0.74
	Pd-N	0.4699	7.1286	0.0756	1.08	0.16	-114.1	0.47
	Pd-Cl	0.4078	3.9819	0.0121	1.20	0.19	-80.6	0.57
3e	Pd-S	0.5310	3.5923	0.0658	1.35	0.25	-102.4	0.69
	Pd-N	0.5495	8.4893	0.0699	1.11	0.16	-143.4	0.53
	Pd-Cl	0.4065	3.9299	0.0129	1.20	0.19	-79.5	0.56
3f	Pd-S	0.5387	3.7203	0.0630	1.35	0.25	-105.5	0.69
	Pd-N	0.4915	7.4909	0.0674	1.09	0.16	-121.4	0.50
	Pd-Cl	0.4081	3.9393	0.0123	1.20	0.19	-79.9	0.57
3g	Pd-S	0.5483	3.7748	0.0618	1.36	0.26	-108.4	0.70
	Pd-N	0.4255	6.3538	0.0703	1.07	0.15	-98.6	0.45
	Pd-Cl	0.4104	3.9558	0.0121	1.20	0.19	-80.6	0.57
3h	Pd-S	0.5181	3.6957	0.0579	1.34	0.24	-101.0	0.67
	Pd-N	0.5235	8.4632	0.0793	1.09	0.15	-137.9	0.49
	Pd-Cl	0.4299	4.0506	0.0109	1.21	0.20	-84.5	0.60
Pd₂[(C₆H₄)PPh₂]₂[N-O]₂								
NO^a	Pd-O	0.5322	10.0157	0.1186	1.04	0.16	-146.4	0.51
	Pd-N	0.5448	8.7295	0.0855	1.10	0.16	-146.2	0.53
Pd₂[(C₆H₄)PPh₂]₂[N-O]₂Cl₂								
NO^a	Pd-O	0.5760	10.3035	0.0514	1.06	0.1961	-156.6	0.53
	Pd-N	0.5198	7.6132	0.0584	1.11	0.1700	-128.6	0.51
	Pd-Cl	0.4196	4.0687	0.0116	1.20	0.1261	-83.5	0.57

^a N-O = 2-hydroxypyridinate

Table S2. Total atomic charges for Pd, S (or O) and N atoms according to the AIM analysis

$\text{Pd}_2[(\text{C}_6\text{H}_5)\text{PPh}_2][\text{N-S}]_2$				$\text{Pd}_2[(\text{C}_6\text{H}_5)\text{PPh}_2][\text{N-S}]_2\text{Cl}_2$				
Complex	q(Pd)	q(N)	q(S/O)	Complex	q(Pd)	q(N)	q(S/O)	q(Cl)
2a	0.331	-1.257	-0.162	3a	0.510	-1.262	-0.089	-0.567
2b	0.340	-1.242	-0.177	3b	0.504	-1.222	-0.104	-0.567
2c	0.338	-1.232	-0.135	3c	0.501	-1.216	-0.095	-0.561
2d	0.324	-1.247	-0.088	3d	0.504	-1.257	-0.018	-0.565
2e	0.352	-1.234	-0.115	3e	0.530	-1.241	-0.016	-0.565
2f	0.354	-1.218	-0.057	3f	0.525	-1.201	0.006	-0.558
2g	0.341	-1.244	0.007	3g	0.504	-1.222	0.045	-0.554
2h	0.362	-0.736	0.020	3h	0.515	-0.744	0.105	-0.529
$\text{Pd}_2[(\text{C}_6\text{H}_5)\text{PPh}_2][\text{N-O}]_2$				$\text{Pd}_2[(\text{C}_6\text{H}_5)\text{PPh}_2][\text{N-O}]_2\text{Cl}_2$				
N-O^a	0.461	-1.270	-1.174	N-O^a	0.642	-1.280	-1.138	-0.562

^aNO = 2-hydroxypyridinate

Table S3. Properties of the frontier molecular orbitals for Pd(II) complexes with N,S ligands. ϵ [eV] = the orbital energy; %Pd= percentage contribution of palladium atomic orbitals in the molecular orbital as calculated by fragment population analysis; %L^P = percentage contribution of the phosphine ligands; %L^{N,S} = percentage contribution of the N,S ligands; %S = contribution of the sulphur atom only; HOMO = highest occupied molecular orbital; LUMO = lowest unoccupied molecular orbital.

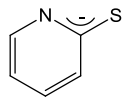
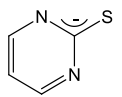
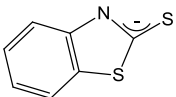
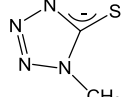
Compound	2a		2d		2g		2h	
N,S-donor ligand								
Frontier molecular orbitals	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
ϵ [eV]	-4.81	-1.12	-4.92	-1.25	-5.10	-1.29	-5.16	-1.28
%Pd	80	50	81	44	77	57	83	62
%L ^P	11	33	10	22	13	31	12	30
%L ^{N,S} (%S)	10 (7)	17 (8)	10 (7)	34 (6)	10 (6)	13 (7)	5 (4)	8 (5)

Table S4. Properties of the frontier molecular orbitals for Pd(III) complexes with N,S ligands. ϵ [eV] = the orbital energy; %Pd= percentage contribution of palladium atomic orbitals in the molecular orbital as calculated by fragment population analysis; %L^P = percentage contribution of the phosphine ligands; %L^{N,S} = percentage contribution of the N,S ligands; %S = contribution of the sulphur atom only; %Cl = percentage contribution of the axial chlorine atoms. HOMO = highest occupied molecular orbital; LUMO = lowest unoccupied molecular orbital.

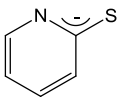
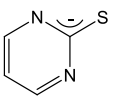
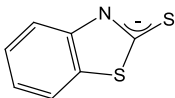
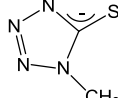
Compound	3a		3d		3g		3h	
N,S-donor ligand								
Frontier molecular orbitals	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
ϵ [eV]	-5.37	-3.26	-5.66	-3.37	-5.51	-3.46	-5.72	-3.43
%Pd	44	65	51	65	30	63	47	62
%L ^P	4	13	4	13	4	15	4	14
%L ^{N,S} (%S)	44 (32)	7 (4)	37 (28)	7 (4)	58 (32)	7 (3)	37 (27)	7 (4)
%Cl	7	15	8	15	8	15	12	17

Table S5. HOMO and LUMO energies and the HOMO-LUMO gaps (eV) for compounds Pd₂[(C₆H₅)PPh₂][N-S]₂, Pd₂[(C₆H₅)PPh₂][N-S]₂Cl₂, Pd₂[(C₆H₅)PPh₂][N-O]₂, and Pd₂[(C₆H₅)PPh₂][N-O]₂Cl₂.

Pd ₂ [(C ₆ H ₅)PPh ₂][N-S] ₂				Pd ₂ [(C ₆ H ₅)PPh ₂][N-S] ₂ Cl ₂			
Complex	HOMO	LUMO	gap	Complex	HOMO	LUMO	gap
2a	-4.81	-1.12	3.69	3a	-5.37	-3.26	2.11
2b	-4.73	-1.13	3.60	3b	-5.24	-3.30	1.94
2c	-4.81	-1.34	3.47	3c	-5.38	-3.29	2.09
2d	-4.92	-1.25	3.67	3d	-5.66	-3.37	2.28
2e	-4.68	-0.93	3.75	3e	-5.06	-3.17	1.89
2f	-4.89	-1.07	3.82	3f	-5.30	-3.27	2.03
2g	-5.10	-1.29	3.80	3g	-5.51	-3.46	2.06
2h	-5.16	-1.28	3.87	3h	-5.72	-3.43	2.29
Pd ₂ [(C ₆ H ₅)PPh ₂][N-O] ₂				Pd ₂ [(C ₆ H ₅)PPh ₂][N-O] ₂ Cl ₂			
N-O^a	-4.79	-1.16	3.63	N-O^a	-5.47	-3.08	1.71

^aNO = 2-hydroxypyridinate

Table S6. Cartesian coordinates of the optimized structures **2a – h** and **3a – h**.

2a

Pd	0.70266500	0.62303600	1.18002500
P	2.17466200	-0.82230100	0.08743300
S	-1.00022100	1.94481700	2.17593000
N	1.61845500	2.45749900	0.43212400
C	-1.67188700	2.87137500	0.85779800
Pd	-0.70280600	0.62310500	-1.18003200
P	-2.17457800	-0.82266300	-0.08744700
S	0.99968600	1.94522100	-2.17600400
N	-1.61885600	2.45750700	-0.43216400
C	-2.32548900	4.08434100	1.17756900
H	-2.35327200	4.39496600	2.21676200
C	-2.89517400	4.85554500	0.18566100
H	-3.39266200	5.78917000	0.43722100
C	-2.80402700	4.42971700	-1.14447000
H	-3.21711300	5.00854700	-1.96411700
C	-2.15387300	3.23693900	-1.39417500
H	-2.03483700	2.86288100	-2.40703000
C	1.67134800	2.87162100	-0.85776100
C	2.32483500	4.08469200	-1.17735000
H	2.35253600	4.39551300	-2.21648400
C	2.89449900	4.85578200	-0.18534000
H	3.39192300	5.78947300	-0.43678300
C	2.80345700	4.42971600	1.14472400
H	3.21653500	5.00842800	1.96445800
C	2.15344500	3.23682400	1.39425000
H	2.03452300	2.86257700	2.40705400
C	1.40946000	-1.53128900	-1.42105900
C	0.25296200	-0.94853700	-1.98158000
C	-0.21029700	-1.46662900	-3.20185200
H	-1.10075400	-1.03864400	-3.65664100
C	0.43041400	-2.52666100	-3.83937000
H	0.04254000	-2.90043700	-4.78470400
C	1.55178200	-3.11911600	-3.25888100
H	2.04924100	-3.95684100	-3.74125700
C	2.03477500	-2.62123300	-2.05374200
H	2.91260200	-3.07487500	-1.59921200
C	3.71436300	0.01846900	-0.46957100
C	4.18928900	-0.05482300	-1.78301800
H	3.62697600	-0.60200200	-2.53250700
C	5.37289700	0.58981200	-2.13952500
H	5.72679400	0.52952000	-3.16564400
C	6.09457500	1.31306100	-1.19238700
H	7.01683200	1.81475100	-1.47476600
C	5.62270600	1.40146200	0.11683700
H	6.17163300	1.97447800	0.85986300
C	4.43526100	0.76658200	0.47249300
H	4.06039300	0.85675400	1.48979400
C	2.82101600	-2.31263800	0.97034800
C	4.14588300	-2.41484800	1.41282700
H	4.85043200	-1.61327400	1.21590100
C	4.58314400	-3.55215200	2.09172700
H	5.61737900	-3.61288600	2.42165400
C	3.70680600	-4.60660300	2.33450700
H	4.05022200	-5.49470500	2.85917900
C	2.38643200	-4.51670100	1.89555900
H	1.69124400	-5.33183400	2.07925400
C	1.94577600	-3.37997700	1.22425500

H	0.91289900	-3.32424300	0.89494600
C	-1.40932000	-1.53162500	1.42103600
C	-0.25291900	-0.94871900	1.98159200
C	0.21041100	-1.46672100	3.20187200
H	1.10080700	-1.03861800	3.65666400
C	-0.43019200	-2.52683100	3.83938700
H	-0.04232600	-2.90053300	4.78475400
C	-1.55146000	-3.11943600	3.25887200
H	-2.04881700	-3.95723200	3.74123200
C	-2.03450100	-2.62163600	2.05371700
H	-2.91223600	-3.07543700	1.59916700
C	-3.71432500	0.01798300	0.46959500
C	-4.43495600	0.76646900	-0.47238600
H	-4.05986900	0.85693200	-1.48956900
C	-5.62243800	1.40132200	-0.11677200
H	-6.17113500	1.97467300	-0.85970700
C	-6.09458900	1.31250800	1.19231900
H	-7.01688400	1.81413400	1.47469200
C	-5.37314600	0.58892500	2.13938700
H	-5.72732500	0.52827800	3.16538800
C	-4.18949500	-0.05564900	1.78293000
H	-3.62730600	-0.60304900	2.53235500
C	-2.82064300	-2.31310800	-0.97040400
C	-4.14547000	-2.41561000	-1.41295800
H	-4.85024300	-1.61423700	-1.21605600
C	-4.58243400	-3.55300600	-2.09190700
H	-5.61664400	-3.61396400	-2.42187600
C	-3.70584900	-4.60725800	-2.33466400
H	-4.04900100	-5.49542300	-2.85939700
C	-2.38553800	-4.51708400	-1.89559800
H	-1.69016100	-5.33206700	-2.07926600
C	-1.94517900	-3.38026900	-1.22424900
H	-0.91235700	-3.32433600	-0.89480200

2b

Pd	0.78831100	-0.55027300	-1.13814900
P	2.20940100	0.90333500	0.00730700
S	-0.94405500	-1.85621000	-2.11937900
N	1.75464600	-2.38212100	-0.44066700
C	-1.67184200	-2.80785300	-0.84489900
Pd	-0.78829000	-0.55013900	1.13816700
S	0.94417100	-1.85598400	2.11941500
P	-2.20938900	0.90331800	-0.00733700
N	-1.75463500	-2.38190300	0.44077800
C	-2.25806100	-4.03264600	-1.22965400
H	-2.16740800	-4.34736100	-2.26359600
C	-2.92555400	-4.79936400	-0.29817300
H	-3.38011100	-5.74410000	-0.58696600
C	-3.00296000	-4.34801000	1.01993700
H	-3.51857600	-4.92273300	1.78286000
C	-2.40337000	-3.14213300	1.35940900
C	-2.45831100	-2.64927500	2.77647900
H	-2.69527100	-1.57973900	2.81896000
H	-1.48271800	-2.77430600	3.26000700
H	-3.20961000	-3.20268800	3.34901000
C	1.67182500	-2.80789700	0.84506600
C	2.25790500	-4.03270800	1.22995300
H	2.16719400	-4.34733700	2.26391500

C	2.92532800	-4.79959400	0.29854100
H	3.37979700	-5.74433500	0.58745200
C	3.00278700	-4.34839400	-1.01960700
H	3.51835500	-4.92323300	-1.78247500
C	1.34940500	1.60592000	1.46610400
C	0.16095600	1.02424100	1.95558400
C	-0.36363900	1.53938200	3.15327000
H	-1.28006600	1.11479900	3.55782200
C	0.24491100	2.59221100	3.83290500
H	-0.19278200	2.96024300	4.75854700
C	1.39690500	3.18536100	3.31712500
H	1.87018500	4.01891100	3.83010400
C	1.94148700	2.69162900	2.13722100
H	2.84480600	3.14389200	1.73400800
C	2.40329000	-3.14249200	-1.35920400
C	2.45823800	-2.64977900	-2.77632800
H	2.69483300	-1.58017500	-2.81887300
H	1.48273400	-2.77518200	-3.25995300
H	3.20978400	-3.20300300	-3.34871100
C	2.88575500	2.40311700	-0.83873400
C	4.23043200	2.52390700	-1.21149700
H	4.93533600	1.73291000	-0.97727400
C	4.68792700	3.66816000	-1.86500000
H	5.73727000	3.74288500	-2.13983500
C	3.81209700	4.71188200	-2.15177000
H	4.17092900	5.60542600	-2.65651600
C	2.47212500	4.60416400	-1.78174600
H	1.77696700	5.41099600	-1.99917800
C	2.01183000	3.46056000	-1.13571200
H	0.96440400	3.39187700	-0.85918900
C	3.72461000	0.08726500	0.66524700
C	4.54132800	-0.62287600	-0.22599000
H	4.26096000	-0.69438200	-1.27394000
C	5.70737400	-1.24323900	0.21612800
H	6.33029400	-1.78649300	-0.48999800
C	6.06357200	-1.17734600	1.56239600
H	6.96892300	-1.66734500	1.91197100
C	5.24765500	-0.49069900	2.45886400
H	5.51051500	-0.44736500	3.51282800
C	4.08499800	0.13787600	2.01601100
H	3.44887200	0.65408900	2.72708900
C	-1.34933700	1.60584600	-1.46613200
C	-0.16090800	1.02410100	-1.95559000
C	0.36373000	1.53916900	-3.15328800
H	1.28015200	1.11452700	-3.55779100
C	-0.24475000	2.59200600	-3.83297000
H	0.19297200	2.95997700	-4.75862000
C	-1.39671600	3.18523300	-3.31721500
H	-1.86995000	4.01879300	-3.83021900
C	-1.94133700	2.69157200	-2.13730100
H	-2.84463600	3.14389800	-1.73411900
C	-2.88584100	2.40309800	0.83861700
C	-2.01192900	3.46051000	1.13576300
H	-0.96446700	3.39181600	0.85938900
C	-2.47228000	4.60408500	1.78180500
H	-1.77712700	5.41088300	1.99938000
C	-3.81230100	4.71181300	2.15166600
H	-4.17117900	5.60532700	2.65643200
C	-4.68810800	3.66812000	1.86473500
H	-5.73748600	3.74285200	2.13942600

C	-4.23055500	2.52388400	1.21124400
H	-4.93543400	1.73289900	0.97691300
C	-3.72456500	0.08718600	-0.66533600
C	-4.08475200	0.13757900	-2.01616100
H	-3.44846900	0.65358200	-2.72725100
C	-5.24738900	-0.49100000	-2.45907500
H	-5.51010200	-0.44781600	-3.51308100
C	-6.06346800	-1.17744900	-1.56261000
H	-6.96880700	-1.66745400	-1.91221100
C	-5.70745400	-1.24314300	-0.21628000
H	-6.33049900	-1.78627200	0.48983000
C	-4.54144400	-0.62276600	0.22590500
H	-4.26124100	-0.69409000	1.27391000

2c

Pd	-0.95020200	-0.24659700	0.99653400
Pd	0.95011600	-0.24659600	-0.99663100
P	-2.17928700	1.21617100	-0.34361400
P	2.17935200	1.21605200	0.34353900
S	0.55642400	-1.59414500	2.24584200
S	-0.55663500	-1.59406300	-2.24588200
N	1.81371400	-2.05972200	-0.12863000
N	-1.81388800	-2.05965700	0.12858600
C	-4.51040600	-0.31556000	-0.44726400
H	-4.36802600	-0.41154400	0.62652100
C	1.10810000	1.91137800	1.65808000
C	0.13733800	1.32121300	-1.95997500
C	-0.13729700	1.32117300	1.95987400
C	-2.96473900	2.71510300	0.40042000
C	2.64168000	-2.81797700	-0.93034500
C	4.51037300	-0.31582000	0.44715200
H	4.36805700	-0.41167900	-0.62665200
C	3.58312700	0.40448300	1.21391800
C	-1.10802400	1.91148500	-1.65815100
C	1.54149000	-2.47302400	1.11500900
C	3.22784100	-4.03245100	-0.47486100
C	-2.64183600	-2.81790900	0.93032300
C	2.96495700	2.71497900	-0.40035000
C	1.58364900	2.99866600	2.41502400
H	2.53323200	3.46002400	2.15350700
C	2.11293000	-3.68541200	1.62723200
H	1.85967200	-3.97642700	2.64091300
C	-3.58316200	0.40476200	-1.21401800
C	-2.11299700	-3.68543400	-1.62720500
H	-1.85972000	-3.97648700	-2.64087300
C	-2.94871700	-2.38052800	2.23987500
H	-2.50013000	-1.45534400	2.59386100
C	2.93095800	-4.44612000	0.85136300
H	3.35869800	-5.37141700	1.23195000
C	3.75891900	0.47338900	2.59996900
H	3.03264500	0.99665700	3.21300800
C	5.60893200	-0.92461800	1.04918100
H	6.31854800	-1.47752800	0.43908300
C	-2.14132100	3.77608200	0.80756500
H	-1.06645800	3.71082200	0.66984700
C	-0.84214800	1.82896600	3.06453200
H	-1.80804600	1.39935100	3.32195300
C	2.94846900	-2.38067600	-2.23994000
H	2.49977400	-1.45557200	-2.59399300

C	-1.54163300	-2.47299000	-1.11503900
C	-1.58347300	2.99885700	-2.41502300
H	-2.53300700	3.46029500	-2.15347500
C	2.14161900	3.77595700	-0.80766700
H	1.06672300	3.71066300	-0.67022600
C	0.84222500	1.82899300	-3.06460800
H	1.80810400	1.39933800	-3.32204300
C	4.07741900	-4.76754000	-1.33003900
H	4.51019000	-5.69500300	-0.96056600
C	4.85454500	-0.14433800	3.20151600
H	4.97544800	-0.08626300	4.28033200
C	-3.75903900	0.47379200	-2.60005100
H	-3.03276500	0.99705000	-3.21309900
C	-4.34695600	2.82814500	0.59580200
H	-5.01077200	2.03219600	0.27401600
C	-3.22790200	-4.03244900	0.47489700
C	4.89098000	3.96986600	-1.18352800
H	5.96731800	4.03920300	-1.32079100
C	-0.35104500	2.88221000	3.83212400
H	-0.92703200	3.24457700	4.68104600
C	4.34722100	2.82807800	-0.59536900
H	5.01097800	2.03212600	-0.27347600
C	-4.85474000	-0.14381400	-3.20158600
H	-4.97569900	-0.08565100	-4.28039000
C	-2.68701800	4.91755100	1.38735800
H	-2.03011100	5.72795300	1.69266700
C	-4.06419400	5.01803900	1.58096800
H	-4.48971300	5.90966500	2.03468800
C	3.78726700	-3.11418400	-3.05370400
H	4.00310100	-2.75700200	-4.05754500
C	-2.93097500	-4.44615900	-0.85130000
H	-3.35865000	-5.37149900	-1.23185100
C	-4.89059100	3.96988300	1.18416700
H	-5.96689500	4.03919300	1.32170600
C	4.06465900	5.01801500	-1.58049500
H	4.49027200	5.90970100	-2.03400900
C	0.86228400	3.48408200	3.49965800
H	1.24618700	4.31879900	4.08080300
C	5.78452800	-0.83733600	2.42969200
H	6.63751500	-1.31775300	2.90260900
C	0.35119300	2.88230800	-3.83215800
H	0.92720500	3.24466100	-4.68106700
C	-0.86207900	3.48426400	-3.49964900
H	-1.24593400	4.31904300	-4.08074200
C	-4.07744400	-4.76754900	1.33010200
H	-4.51013400	-5.69506600	0.96067400
C	-5.60904600	-0.92422800	-1.04927600
H	-6.31865900	-1.47713900	-0.43917700
C	-3.78748000	-3.11404700	3.05365900
H	-4.00338100	-2.75680600	4.05746500
C	4.35794800	-4.32035800	-2.60302900
H	5.01314400	-4.89132600	-3.25531400
C	-5.78472700	-0.83681800	-2.42976600
H	-6.63777600	-1.31713700	-2.90267300
C	-4.35804200	-4.32030700	2.60305500
H	-5.01320100	-4.89129200	3.25536400
C	2.68743000	4.91747500	-1.38725000
H	2.03057700	5.72786500	-1.69270600

2d

Pd	0.68732300	0.62729300	1.18359400
P	2.17043000	-0.82234000	0.10103900
S	-0.98451300	1.96382600	2.19809000
N	1.60068900	2.45946400	0.40871100
C	-1.69476600	2.86198900	0.89098500
Pd	-0.68723400	0.62750300	-1.18358100
P	-2.17048100	-0.82220800	-0.10104500
S	0.98469300	1.96386400	-2.19808000
N	-1.60044500	2.45978000	-0.40867900
C	-2.90704800	4.72406700	0.32193600
H	-3.44943200	5.60489500	0.66591600
C	-2.79216700	4.43567800	-1.03911300
H	-3.20576400	5.07514100	-1.81062800
C	-2.12058300	3.26735400	-1.34726200
H	-1.98057800	2.94080100	-2.37405800
C	1.69505000	2.86181600	-0.89090500
C	2.90778600	4.72354200	-0.32168300
H	3.45039000	5.60426900	-0.66557700
C	2.79273200	4.43510800	1.03935200
H	3.20639000	5.07445000	1.81093600
C	2.12095600	3.26687300	1.34738500
H	1.98090100	2.94024100	2.37415300
C	1.42338800	-1.52081100	-1.42079200
C	0.27305700	-0.93593600	-1.99112700
C	-0.17922900	-1.44755600	-3.21785200
H	-1.06408500	-1.01613900	-3.68010900
C	0.46711700	-2.50572600	-3.85262300
H	0.08844900	-2.87570000	-4.80309300
C	1.58354600	-3.09995800	-3.26426100
H	2.08597600	-3.93503800	-3.74593100
C	2.05562300	-2.60722700	-2.05283300
H	2.92987500	-3.06189400	-1.59256600
C	3.71077900	0.02996000	-0.43314300
C	4.18075000	-0.00225600	-1.74991900
H	3.61693000	-0.52766200	-2.51372200
C	5.36149400	0.65634700	-2.09082200
H	5.71005100	0.63089600	-3.12000500
C	6.08549700	1.35084100	-1.12463200
H	7.00512700	1.86344200	-1.39526700
C	5.61886300	1.39800700	0.18890400
H	6.17144300	1.94687700	0.94737500
C	4.43337000	0.75130000	0.52910200
H	4.06311700	0.80713200	1.55096600
C	2.80761400	-2.31755800	0.98074300
C	4.13583200	-2.43736900	1.40833400
H	4.84872700	-1.64500700	1.20452600
C	4.56533800	-3.58125600	2.08117200
H	5.60212300	-3.65601200	2.39988900
C	3.67785900	-4.62433600	2.33213400
H	4.01515800	-5.51733900	2.85235900
C	2.35423900	-4.51711400	1.90692900
H	1.65074900	-5.32365600	2.09664400
C	1.92124700	-3.37402400	1.24156200
H	0.88605400	-3.30506100	0.92224400
C	-1.42361700	-1.52071300	1.42088300
C	-0.27319200	-0.93599900	1.99120500
C	0.17893800	-1.44754000	3.21801600
H	1.06383300	-1.01622200	3.68028200

C	-0.46764200	-2.50551400	3.85288600
H	-0.08909600	-2.87545500	4.80341800
C	-1.58415500	-3.09959600	3.26454300
H	-2.08676200	-3.93452700	3.74629000
C	-2.05608700	-2.60692600	2.05303000
H	-2.93042000	-3.06147300	1.59279800
C	-3.71085400	0.03020300	0.43290100
C	-4.43334600	0.75147200	-0.52947500
H	-4.06301900	0.80719800	-1.55131200
C	-5.61882700	1.39827700	-0.18942200
H	-6.17131300	1.94712000	-0.94798000
C	-6.08554100	1.35129300	1.12409300
H	-7.00516000	1.86397200	1.39462500
C	-5.36164400	0.65686300	2.09040700
H	-5.71028200	0.63154400	3.11956500
C	-4.18092100	-0.00185100	1.74964800
H	-3.61719400	-0.52725900	2.51352200
C	-2.80775500	-2.31739100	-0.98071900
C	-4.13606600	-2.43731900	-1.40797400
H	-4.84897600	-1.64503900	-1.20393200
C	-4.56563100	-3.58121500	-2.08076100
H	-5.60250100	-3.65607300	-2.39918400
C	-3.67809400	-4.62416500	-2.33205500
H	-4.01541900	-5.51714300	-2.85229700
C	-2.35436400	-4.51681700	-1.90722600
H	-1.65082500	-5.32325800	-2.09721100
C	-1.92132700	-3.37372600	-1.24188100
H	-0.88605400	-3.30467700	-0.92284500
N	2.36625200	3.97054100	-1.26531900
N	-2.36563100	3.97088100	1.26550600

2e

Pd	-0.64475200	-0.58022800	1.24398500
P	-2.14181800	0.85959000	0.19013500
S	1.07901500	-1.92833900	2.21323600
N	1.56546400	-2.35782800	-0.48391700
C	1.61971900	-2.76539600	0.79095400
Pd	0.64470900	-0.58015300	-1.24400300
P	2.14173900	0.85970000	-0.19022700
S	-1.07908600	-1.92830700	-2.21317800
C	2.12013900	-3.35223600	-1.25500200
H	2.15791000	-3.26779500	-2.33124700
C	2.48299900	-4.75647300	2.03904600
H	1.65584000	-4.62105700	2.74026300
H	3.40875900	-4.42183700	2.51997400
H	2.57253200	-5.81392700	1.77840900
C	-1.61950800	-2.76559200	-0.79091800
C	2.54124200	-4.36786100	-0.45052700
H	3.02818400	-5.30750000	-0.66532300
N	2.21426900	-3.99642900	0.83892200
C	-2.48229400	-4.75691400	-2.03897900
H	-2.57056300	-5.81452300	-1.77852100
H	-1.65565100	-4.62047200	-2.74059800
H	-3.40866900	-4.42315600	-2.51933000
N	-1.56544800	-2.35796100	0.48394400
C	-2.11986600	-3.35251000	1.25503200
H	-2.15770700	-3.26805200	2.33127200
C	-2.54061800	-4.36829100	0.45057200
H	-3.02718800	-5.30812000	0.66538500

N	-2.21365400	-3.99682300	-0.83886800
C	-1.46296900	1.58156300	-1.35411700
C	-0.34710900	0.99571800	-1.98921700
C	0.04067000	1.51934900	-3.23366400
H	0.89827300	1.08881700	-3.74586600
C	-0.63291100	2.58595200	-3.82385800
H	-0.30403600	2.96357400	-4.78991300
C	-1.71192100	3.18132100	-3.17000600
H	-2.23356400	4.02517100	-3.61486200
C	-2.12155300	2.67870900	-1.93994400
H	-2.96629500	3.13486600	-1.42893200
C	-3.70497400	0.01575600	-0.29461700
C	-4.36352000	-0.75862600	0.67111100
H	-3.92090200	-0.87759900	1.65728600
C	-5.57090000	-1.38640800	0.37515400
H	-6.07139200	-1.97910600	1.13681800
C	-6.12509200	-1.26563600	-0.89901900
H	-7.06458300	-1.75989300	-1.13443700
C	-5.46458600	-0.51785100	-1.87134700
H	-5.88318800	-0.43103500	-2.87098700
C	-4.26109100	0.12045000	-1.57346700
H	-3.74859500	0.68939300	-2.34216700
C	-2.75341000	2.33858700	1.11620700
C	-1.87898800	3.41668600	1.32205000
H	-0.86832400	3.37728200	0.92776400
C	-2.29199800	4.54251700	2.02831900
H	-1.59806800	5.36640000	2.17388200
C	-3.58268400	4.60998200	2.55149900
H	-3.90430500	5.48930700	3.10410100
C	-4.45777000	3.54442100	2.35703900
H	-5.46942600	3.58769500	2.75317600
C	-4.04874300	2.41838400	1.64268300
H	-4.75224500	1.60706700	1.48525900
C	1.46289600	1.58155800	1.35408600
C	0.34703400	0.99568800	1.98915600
C	-0.04077900	1.51931000	3.23359600
H	-0.89840200	1.08877800	3.74576700
C	0.63278400	2.58590700	3.82382100
H	0.30387600	2.96351800	4.78986900
C	1.71180900	3.18128400	3.17000600
H	2.23345300	4.02511900	3.61489000
C	2.12145700	2.67870100	1.93993700
H	2.96620000	3.13487700	1.42894600
C	2.75324000	2.33883700	-1.11614000
C	1.87867300	3.41683100	-1.32196700
H	0.86796300	3.37721600	-0.92782700
C	2.29160800	4.54282100	-2.02802000
H	1.59756900	5.36661300	-2.17358100
C	3.58236900	4.61056600	-2.55099400
H	3.90393000	5.49002200	-3.10342200
C	4.45759500	3.54512600	-2.35653800
H	5.46930800	3.58861400	-2.75250800
C	4.04863900	2.41892300	-1.64239500
H	4.75225400	1.60770300	-1.48497800
C	3.70494200	0.01587200	0.29440900
C	4.36358100	-0.75827900	-0.67144100
H	3.92102000	-0.87708800	-1.65766800
C	5.57098700	-1.38604200	-0.37555600
H	6.07155800	-1.97854800	-1.13731800
C	6.12511500	-1.26549300	0.89866900

H	7.06463200	-1.75973100	1.13402400
C	5.46451000	-0.51795800	1.87111700
H	5.88305100	-0.43132300	2.87079900
C	4.26098400	0.12032700	1.57331000
H	3.74841700	0.68908300	2.34209900

2f

Pd	-0.81780600	-0.11554200	1.13448600
S	0.76726100	-1.46927300	2.31588300
P	-2.16156400	1.32387100	-0.10789900
N	2.16379800	-3.50910200	1.18382100
C	1.53131200	-2.29705300	1.00742500
Pd	0.81760900	-0.11477200	-1.13462800
P	2.16047300	1.32530900	0.10764600
S	-0.76664000	-1.46963900	-2.31598000
N	1.65037000	-1.88794300	-0.26119900
C	2.25131700	-4.26431500	2.41171000
H	1.47163000	-3.91625200	3.09177900
H	3.22870700	-4.13066200	2.88942900
H	2.09459000	-5.32604200	2.19802000
N	-1.64911100	-1.88954800	0.26115100
C	2.71687800	-3.87998000	-0.02712800
N	-2.16055700	-3.51124500	-1.18396200
C	3.46780200	-4.98834200	-0.40953700
H	3.74005000	-5.76680100	0.29770600
C	3.86301900	-5.05527500	-1.74457000
H	4.44950900	-5.90538800	-2.08293500
C	3.51792300	-4.04657700	-2.65771000
H	3.83992700	-4.13402300	-3.69221500
C	2.76827900	-2.93926300	-2.26805400
H	2.48464200	-2.16327700	-2.97311400
C	2.36901900	-2.85932100	-0.93304500
C	-1.52957400	-2.29844800	-1.00749500
C	-2.24734000	-4.26616300	-2.41209200
H	-1.46604200	-3.91926300	-3.09092300
H	-3.22374500	-4.13101100	-2.89140500
H	-2.09257200	-5.32811400	-2.19815300
C	-1.26131400	2.04808000	-1.53251100
C	-0.06524600	1.46499800	-2.00140700
C	0.49477700	1.99222300	-3.17722500
H	1.41847800	1.56626700	-3.56308200
C	-0.08998000	3.05856600	-3.85646300
H	0.37306600	3.43746700	-4.76523200
C	-1.25138000	3.65204800	-3.36177800
H	-1.70519900	4.49634500	-3.87476300
C	-1.83036200	3.14655600	-2.20338800
H	-2.73943300	3.60136000	-1.81661600
C	-2.90461900	2.79884800	0.72133500
C	-4.26456300	2.87215700	1.04779600
H	-4.93258400	2.05748900	0.78755300
C	-4.78124100	3.99684700	1.69073900
H	-5.84105200	4.03577700	1.93030400
C	-3.94979800	5.06646900	2.01271300
H	-4.35480900	5.94499800	2.50878900
C	-2.59450100	5.00412100	1.69093200
H	-1.93403000	5.83123000	1.93818800
C	-2.07478200	3.87997200	1.05595300
H	-1.01590200	3.84499700	0.81867600
C	-3.63002700	0.47432900	-0.82260000

C	-3.98823000	0.58635200	-2.17010600
H	-3.37086900	1.16542600	-2.84888900
C	-5.12590500	-0.06035900	-2.65136100
H	-5.38953200	0.03174600	-3.70208600
C	-5.91573300	-0.82535700	-1.79577000
H	-6.80181000	-1.32903100	-2.17449100
C	-5.55904900	-0.95271200	-0.45352600
H	-6.15738200	-1.56220600	0.21856300
C	-4.41880600	-0.31374000	0.02745900
H	-4.13055700	-0.44208900	1.06798600
C	1.25982600	2.04860000	1.53252500
C	0.06397100	1.46483400	2.00114500
C	-0.49653300	1.99164700	3.17692500
H	-1.42013300	1.56524800	3.56253200
C	0.08764400	3.05812200	3.85646200
H	-0.37575700	3.43668800	4.76518700
C	1.24891000	3.65215000	3.36213600
H	1.70230900	4.49651900	3.87538100
C	1.82827900	3.14716800	2.20371600
H	2.73718100	3.60249400	1.81717800
C	2.90256600	2.80119300	-0.72095800
C	2.07161200	3.88135600	-1.05595700
H	1.01260100	3.84494100	-0.81953500
C	2.59039100	5.00635400	-1.69019100
H	1.92904900	5.83265600	-1.93783700
C	3.94589600	5.07055400	-2.01076400
H	4.35020000	5.94975800	-2.50621900
C	4.77844600	4.00194000	-1.68837200
H	5.83841300	4.04234000	-1.92699400
C	4.26267900	2.87636500	-1.04621100
H	4.93155200	2.06248500	-0.78568500
C	3.62951700	0.47650500	0.82205800
C	3.98696500	0.58747400	2.16985600
H	3.36884200	1.16544400	2.84888600
C	5.12492100	-0.05880600	2.65103200
H	5.38796300	0.03245600	3.70197500
C	5.91579000	-0.82231200	1.79508100
H	6.80208500	-1.32565400	2.17374400
C	5.55985500	-0.94864600	0.45253300
H	6.15900900	-1.55700800	-0.21984900
C	4.41933100	-0.31013100	-0.02836600
H	4.13163900	-0.43776800	-1.06913600
C	-2.36659900	-2.86182600	0.93293100
C	-2.71331400	-3.88281100	0.02693400
C	-3.46302900	-4.99202400	0.40926400
H	-3.73450200	-5.77069000	-0.29804400
C	-3.85816400	-5.05950800	1.74428600
H	-4.44370700	-5.91030100	2.08257900
C	-3.51418300	-4.05050300	2.65751600
H	-3.83611300	-4.13836900	3.69201100
C	-2.76577000	-2.94233700	2.26793200
H	-2.48303200	-2.16608300	2.97305000

2g

Pd	-0.87646200	-0.17138500	1.08144000
S	0.64364000	-1.54881700	2.31173100
P	-2.16172700	1.28800000	-0.21036300
C	1.52025100	-2.34246000	1.06622900
Pd	0.87627000	-0.17140300	-1.08138200

P	2.16236700	1.28706600	0.21046600
S	-0.64476700	-1.54779300	-2.31160800
N	1.71369300	-1.95725600	-0.18319800
N	-1.71505200	-1.95655800	0.18320400
C	2.98219600	-3.94153500	-0.15196800
C	3.81915300	-4.90084100	-0.71872600
H	4.17151400	-5.74678800	-0.13545300
C	4.18920500	-4.74973400	-2.05179400
H	4.83740500	-5.48913800	-2.51434500
C	3.72912700	-3.65888500	-2.80133300
H	4.02246900	-3.56147800	-3.84319800
C	2.89521100	-2.70177600	-2.23578400
H	2.52215500	-1.86118800	-2.81384200
C	2.51602900	-2.83887200	-0.89554300
C	-1.52144400	-2.34161900	-1.06625800
C	-1.18756500	1.98698200	-1.59727900
C	0.02811900	1.39589400	-1.99912000
C	0.65122100	1.90670900	-3.14994600
H	1.59282500	1.47431200	-3.48148100
C	0.10565800	2.96618000	-3.87089200
H	0.61589400	3.33262700	-4.75910100
C	-1.07763800	3.56844500	-3.44342400
H	-1.50206100	4.40720500	-3.98938000
C	-1.71677700	3.07931300	-2.31013500
H	-2.64258900	3.54165800	-1.97582000
C	-2.91298400	2.78056800	0.57763300
C	-4.28666300	2.89122000	0.82673900
H	-4.96121400	2.09454800	0.53045300
C	-4.80775800	4.03165000	1.43767100
H	-5.87781200	4.09979200	1.61742000
C	-3.96716700	5.07970000	1.80347300
H	-4.37543200	5.97023500	2.27472700
C	-2.59827300	4.98073200	1.55698900
H	-1.93079400	5.79106400	1.83841600
C	-2.07438000	3.84092600	0.95439900
H	-1.00538600	3.77712200	0.77602700
C	-3.60563900	0.45082100	-0.98329300
C	-3.86989700	0.51262100	-2.35557800
H	-3.19351500	1.04607300	-3.01514900
C	-4.99082700	-0.12595300	-2.88446500
H	-5.18006500	-0.07592400	-3.95368900
C	-5.85769700	-0.83081000	-2.05270700
H	-6.72925400	-1.32944800	-2.46924300
C	-5.59470300	-0.90864600	-0.68529100
H	-6.25384200	-1.47225000	-0.03036700
C	-4.47083900	-0.27953200	-0.15582700
H	-4.25864700	-0.36761200	0.90704800
C	1.18839300	1.98633400	1.59731500
C	-0.02732900	1.39540600	1.99920600
C	-0.65019000	1.90615500	3.15022000
H	-1.59177200	1.47381300	3.48188200
C	-0.10441200	2.96548300	3.87119500
H	-0.61446200	3.33188800	4.75953000
C	1.07890900	3.56765400	3.44362300
H	1.50347800	4.40633300	3.98958700
C	1.71786100	3.07851100	2.31024900
H	2.64374700	3.54069800	1.97590200
C	2.91449400	2.77918600	-0.57750900
C	2.07665500	3.84019900	-0.95412900
H	1.00762500	3.77724300	-0.77561000

C	2.60134300	4.97959400	-1.55680300
H	1.93445600	5.79047000	-1.83805800
C	3.97026500	5.07749300	-1.80355800
H	4.37913400	5.96771600	-2.27487800
C	4.81009900	4.02877400	-1.43792800
H	5.88017000	4.09604700	-1.61790000
C	4.28821000	2.88876500	-0.82689000
H	4.96219900	2.09158300	-0.53069300
C	3.60570200	0.44912600	0.98361800
C	3.87011900	0.51115500	2.35585600
H	3.19411800	1.04519700	3.01534200
C	4.99070000	-0.12796400	2.88481600
H	5.18006500	-0.07775300	3.95401000
C	5.85706100	-0.83359000	2.05317500
H	6.72835400	-1.33263300	2.46977600
C	5.59391500	-0.91163300	0.68580200
H	6.25264700	-1.47583100	0.03097700
C	4.47039300	-0.28196400	0.15626200
H	4.25808000	-0.37016600	-0.90657900
C	-2.51758700	-2.83820900	0.89526300
C	-2.98373600	-3.94070800	0.15143800
C	-3.82099400	-4.89993100	0.71789200
H	-4.17335700	-5.74576300	0.13444900
C	-4.19129800	-4.74893800	2.05090000
H	-4.83977000	-5.48826600	2.51319200
C	-3.73118700	-3.65827500	2.80069900
H	-4.02472000	-3.56099500	3.84252000
C	-2.89700400	-2.70123000	2.23545300
H	-2.52386300	-1.86078800	2.81367700
S	-2.34243500	-3.85354800	-1.46832300
S	2.34125700	-3.85456500	1.46795000

2h

Pd	0.65631300	-0.59943800	-1.24818600
S	-0.99656000	-2.02177600	-2.26089400
P	2.12695200	0.86575400	-0.19423900
N	1.60533500	-2.33711200	-0.43295200
C	-1.63595100	-2.75093500	-0.84482800
Pd	-0.65646800	-0.59944000	1.24806400
P	-2.12700300	0.86564300	0.19402100
S	0.99652400	-2.02163600	2.26100200
N	-1.60525500	-2.33737200	0.43306800
C	1.63614700	-2.75062200	0.84495100
N	2.26171400	-3.24370400	-1.18333400
C	2.66288400	-4.78323700	1.92447800
H	1.76256300	-4.99172100	2.50847300
H	3.40752200	-4.30847100	2.57014000
H	3.06615300	-5.70514800	1.50471600
N	2.70891900	-4.19207600	-0.44634600
C	-2.66198100	-4.78398400	-1.92423600
H	-1.76153100	-4.99240700	-2.50805400
H	-3.40660400	-4.30944500	-2.57008300
H	-3.06516000	-5.70590700	-1.50441900
N	2.32833800	-3.91363300	0.82140400
N	-2.26145500	-3.24406500	1.18347000
N	-2.70825200	-4.19267600	0.44653900
N	-2.32775800	-3.91417000	-0.82123100
C	1.44555200	1.56718400	1.35663900
C	0.34378500	0.96408200	1.99912400

C	-0.03858600	1.46885300	3.25239700
H	-0.88472200	1.02219200	3.76964800
C	0.62829300	2.53818700	3.84489800
H	0.30527200	2.90236000	4.81781600
C	1.69302700	3.15278700	3.18514900
H	2.20848100	3.99894000	3.63249400
C	2.09707200	2.66666200	1.94703700
H	2.93138300	3.13712800	1.43203600
C	3.68885800	0.01823600	0.28301900
C	4.25119300	0.12697100	1.55923900
H	3.74688000	0.70358000	2.32776100
C	5.45247000	-0.51715000	1.85420400
H	5.87687900	-0.42757300	2.85107900
C	6.10272100	-1.27411700	0.88202400
H	7.03904900	-1.77484300	1.11569100
C	5.54188500	-1.39843000	-0.38907700
H	6.03104700	-2.00225400	-1.14874400
C	4.33795000	-0.76376400	-0.68424600
H	3.88955100	-0.89265000	-1.66654100
C	2.72495000	2.34634200	-1.12055000
C	4.02036600	2.42956000	-1.64621600
H	4.72580600	1.61971200	-1.49028000
C	4.42499200	3.55764100	-2.35954700
H	5.43599200	3.60463500	-2.75646800
C	3.54575800	4.62001900	-2.55282900
H	3.86428500	5.50072200	-3.10482700
C	2.25495000	4.54806200	-2.03041000
H	1.55857400	5.36982800	-2.17570800
C	1.84552700	3.42029400	-1.32529600
H	0.83443400	3.37624800	-0.93257300
C	-1.44558000	1.56725700	-1.35676200
C	-0.34397400	0.96397000	-1.99938100
C	0.03829500	1.46867600	-3.25270800
H	0.88420500	1.02179300	-3.77013900
C	-0.62840400	2.53821000	-3.84505900
H	-0.30541000	2.90237600	-4.81798900
C	-1.69287700	3.15305400	-3.18512000
H	-2.20815400	3.99938800	-3.63232800
C	-2.09691300	2.66691900	-1.94700700
H	-2.93108800	3.13750000	-1.43189500
C	-2.72501400	2.34602600	1.12066700
C	-4.02011400	2.42863800	1.64720900
H	-4.72533700	1.61853300	1.49160300
C	-4.42472000	3.55642800	2.36101200
H	-5.43547400	3.60294400	2.75861000
C	-3.54578000	4.61911800	2.55391300
H	-3.86428500	5.49958800	3.10629700
C	-2.25528900	4.54777200	2.03062600
H	-1.55915100	5.36979300	2.17562600
C	-1.84588500	3.42029600	1.32504300
H	-0.83504000	3.37672400	0.93162300
C	-3.68895800	0.01828400	-0.28343500
C	-4.25154000	0.12767300	-1.55949200
H	-3.74733900	0.70459800	-2.32784900
C	-5.45290000	-0.51624500	-1.85454000
H	-5.87749900	-0.42616600	-2.85129100
C	-6.10300300	-1.27366100	-0.88260600
H	-7.03938600	-1.77424100	-1.11636600
C	-5.54195300	-1.39859500	0.38833200
H	-6.03101500	-2.00273200	1.14781500

C	-4.33793700	-0.76410900	0.68358700
H	-3.88941100	-0.89342700	1.66576400

3a

Pd	0.78185500	0.48168200	1.04013800
P	2.26992200	-0.86048600	-0.17217000
S	-0.84865100	1.68521100	2.27379500
N	1.53621800	2.42132300	0.23498600
C	-1.53818400	2.74615500	1.07787400
Pd	-0.78179200	0.48173200	-1.04014600
P	-2.26992300	-0.86042100	0.17214600
S	0.84884500	1.68518800	-2.27373500
N	-1.53607200	2.42138700	-0.23491100
C	-2.09252800	3.96644800	1.51450700
H	-2.07989400	4.19114000	2.57601500
C	-2.60381600	4.86030900	0.59413800
H	-3.02790100	5.80502500	0.92562500
C	-2.53539900	4.54274700	-0.76471200
H	-2.89656800	5.21994000	-1.53173700
C	-1.99234400	3.32348600	-1.12819300
H	-1.92890900	3.01975800	-2.16599700
C	1.53833300	2.74613100	-1.07778600
C	2.09264800	3.96645100	-1.51438000
H	2.08001400	4.19117700	-2.57588000
C	2.60391600	4.86029200	-0.59397900
H	3.02797900	5.80502700	-0.92543500
C	2.53550400	4.54268300	0.76485700
H	2.89665700	5.21985800	1.53190600
C	1.99246600	3.32340100	1.12830200
H	1.92903800	3.01964100	2.16610000
C	1.35840300	-1.67277900	-1.51095900
C	0.08403300	-1.19577800	-1.87624400
C	-0.56669100	-1.83869200	-2.93762300
H	-1.54517700	-1.49903800	-3.25178000
C	0.02795700	-2.90233900	-3.61579100
H	-0.51001100	-3.36642700	-4.43924800
C	1.28649300	-3.36948200	-3.24805500
H	1.75021200	-4.19970200	-3.77454100
C	1.94421900	-2.75516000	-2.19089600
H	2.92222700	-3.11401700	-1.87979200
C	3.67809200	0.05257600	-0.91484500
C	4.03982100	-0.13131500	-2.25498700
H	3.45180200	-0.78018000	-2.89560500
C	5.14466200	0.53591600	-2.77862600
H	5.41410500	0.38784800	-3.82121500
C	5.89321100	1.39507300	-1.97582800
H	6.75421200	1.91495900	-2.38862800
C	5.52730700	1.59352200	-0.64588700
H	6.09713800	2.27159000	-0.01579400
C	4.42135400	0.93253200	-0.11504900
H	4.12621800	1.10443200	0.91729800
C	3.06051500	-2.23337300	0.76008700
C	4.30950300	-2.06997300	1.37265800
H	4.84106400	-1.12900600	1.28880900
C	4.88603400	-3.11610100	2.08914700
H	5.85698100	-2.97216900	2.55568800
C	4.22543400	-4.33716400	2.20554500
H	4.68002400	-5.15365400	2.76095200
C	2.97877300	-4.50643200	1.60591500

H	2.45236800	-5.45335200	1.69342600
C	2.39584900	-3.46097200	0.89481500
H	1.42225400	-3.60379000	0.43719700
C	-1.35842500	-1.67277900	1.51090600
C	-0.08404700	-1.19580800	1.87621500
C	0.56665700	-1.83877400	2.93757300
H	1.54514900	-1.49914900	3.25173800
C	-0.02800600	-2.90243600	3.61570000
H	0.50995700	-3.36655900	4.43914000
C	-1.28654900	-3.36954800	3.24794300
H	-1.75027400	-4.19979200	3.77438600
C	-1.94426200	-2.75517200	2.19080600
H	-2.92227100	-3.11400700	1.87967800
C	-3.67808400	0.05265800	0.91479400
C	-4.42133900	0.93257600	0.11495000
H	-4.12617600	1.10445000	-0.91739400
C	-5.52730500	1.59358200	0.64574300
H	-6.09713000	2.27162300	0.01561600
C	-5.89322900	1.39517200	1.97568100
H	-6.75424200	1.91506300	2.38845000
C	-5.14469700	0.53603800	2.77852400
H	-5.41416200	0.38801300	3.82111500
C	-4.03984500	-0.13120500	2.25493300
H	-3.45183900	-0.78006400	2.89557200
C	-3.06062900	-2.23323000	-0.76012400
C	-4.30959500	-2.06970000	-1.37270400
H	-4.84103600	-1.12866400	-1.28887800
C	-4.88623900	-3.11577500	-2.08917200
H	-5.85716500	-2.97174200	-2.55572600
C	-4.22578300	-4.33692200	-2.20552600
H	-4.68046800	-5.15336900	-2.76091700
C	-2.97914700	-4.50632400	-1.60588000
H	-2.45285400	-5.45331000	-1.69334900
C	-2.39610700	-3.46091200	-0.89480300
H	-1.42253100	-3.60383700	-0.43717500
Cl	2.45020800	0.70772600	2.87557200
Cl	-2.45017200	0.70791400	-2.87544000

3b

Pd	0.77831400	-0.41236700	-1.03184300
P	2.28254300	0.94971700	0.17207900
S	-1.01836600	-1.41181500	-2.19975700
N	1.53472600	-2.46538800	-0.23648200
C	-1.66336000	-2.60388600	-1.10180800
Pd	-0.78187400	-0.42049600	1.03516700
S	1.01194100	-1.40858100	2.21253800
P	-2.29904900	0.92546900	-0.17264000
N	-1.50169800	-2.50029500	0.24078000
C	-2.36447900	-3.66848700	-1.69420500
H	-2.47187900	-3.68919900	-2.77348300
C	-2.88273500	-4.66294400	-0.89041100
H	-3.44471300	-5.48859100	-1.32023700
C	-2.62183100	-4.61234200	0.47481300
H	-2.95051300	-5.40830600	1.13521500
C	-1.90143200	-3.54716800	1.01657100
C	-1.49741400	-3.65405500	2.45731900
H	-1.49314400	-2.69753800	2.97340200
H	-0.48596200	-4.07515700	2.51252700
H	-2.17324600	-4.33745700	2.98073100

C	1.70076500	-2.56795600	1.10719800
C	2.43866900	-3.61045000	1.69331400
H	2.54891700	-3.63223600	2.77237200
C	2.99164800	-4.58298000	0.88452400
H	3.58189300	-5.39037500	1.31110400
C	2.73115900	-4.53397500	-0.47981200
H	3.08770000	-5.31358200	-1.14590600
C	1.33448700	1.77070800	1.48588800
C	0.05660800	1.29099600	1.83924900
C	-0.61516600	1.92996100	2.88651200
H	-1.59229400	1.57925600	3.19228300
C	-0.04112000	3.00673900	3.56387500
H	-0.59504500	3.46893100	4.37759800
C	1.21386600	3.48610400	3.20557900
H	1.66178200	4.32682600	3.72904100
C	1.89256500	2.86863800	2.16226900
H	2.86898500	3.23890400	1.86022800
C	1.97376000	-3.49131800	-1.01607800
C	1.58377300	-3.61477400	-2.46079900
H	1.26285100	-2.67950300	-2.90543600
H	0.75719700	-4.33433600	-2.53532900
H	2.42153200	-4.01010100	-3.04395100
C	3.05540300	2.33640800	-0.76140700
C	4.30321300	2.17860000	-1.37890300
H	4.83448100	1.23684500	-1.30310000
C	4.87712100	3.22878400	-2.09113700
H	5.84673100	3.08772600	-2.56139100
C	4.21560100	4.45027500	-2.19916000
H	4.66827200	5.27031700	-2.75097800
C	2.97060100	4.61480500	-1.59530400
H	2.44277500	5.56160200	-1.67595500
C	2.39052600	3.56455800	-0.88836700
H	1.41781200	3.70496000	-0.42851600
C	3.72591100	0.10065600	0.92908100
C	4.46077200	-0.80811800	0.15589100
H	4.13231500	-1.04617200	-0.85282500
C	5.60509400	-1.40680300	0.68176000
H	6.16837100	-2.10785700	0.07120200
C	6.01760000	-1.11635200	1.97990900
H	6.90902600	-1.58597300	2.38840500
C	5.27559300	-0.22844000	2.75858700
H	5.58120700	-0.00849400	3.77838500
C	4.13423900	0.37697200	2.23981200
H	3.55266800	1.04777700	2.86366900
C	-1.35854000	1.75696200	-1.48598600
C	-0.07601500	1.28954400	-1.83907200
C	0.58953000	1.93328900	-2.88731600
H	1.56962700	1.59069200	-3.19310800
C	0.00538700	3.00430100	-3.56525500
H	0.55437700	3.47084300	-4.37983900
C	-1.25349000	3.47276500	-3.20614800
H	-1.70906800	4.30931600	-3.72970200
C	-1.92651400	2.84971900	-2.16236500
H	-2.90603600	3.21148600	-1.86013200
C	-3.08788400	2.30461100	0.75891700
C	-2.43543200	3.53904400	0.88902700
H	-1.46242100	3.68916200	0.43286000
C	-3.02828500	4.58328900	1.59428800
H	-2.50993800	5.53510500	1.67742100
C	-4.27397000	4.40646500	2.19323600

H	-4.73664800	5.22179300	2.74374300
C	-4.92331700	3.17873000	2.08193800
H	-5.89334300	3.02806400	2.54834500
C	-4.33655500	2.13453800	1.37141300
H	-4.85815400	1.18756600	1.29298100
C	-3.73356200	0.06138900	-0.93012200
C	-4.14980900	0.34092300	-2.23774700
H	-3.57956300	1.02399500	-2.85877100
C	-5.28353000	-0.27735700	-2.75777400
H	-5.59504900	-0.05477900	-3.77521700
C	-6.01016500	-1.18181100	-1.98357000
H	-6.89546300	-1.66195900	-2.39313200
C	-5.59019700	-1.47467800	-0.68841700
H	-6.14171800	-2.18776300	-0.08105600
C	-4.45355700	-0.86259100	-0.16106400
H	-4.12059800	-1.10120300	0.84593100
Cl	2.53041500	-0.56041200	-2.80585900
Cl	-2.54123500	-0.57078200	2.80639200

3c

Pd	-0.87948000	-0.05921500	0.94896100
Pd	0.88010100	-0.06055900	-0.94928300
P	-2.26169300	1.29809800	-0.38912800
P	2.26398600	1.29493500	0.38905800
S	0.75638900	-1.08173300	2.31337100
S	-0.75642800	-1.08147900	-2.31404300
N	1.55742300	-2.11146100	-0.05631000
N	-1.55991900	-2.10810900	0.05614700
C	-4.39101400	-0.50966300	-0.58816100
H	-4.15237800	-0.75308700	0.44426900
C	1.19984500	2.11915600	1.60709300
C	0.10947900	1.64244000	-1.83988700
C	-0.10675200	1.64280200	1.83959700
C	-3.13336700	2.67469400	0.46419300
C	2.08575100	-3.15862700	-0.79921800
C	4.39010000	-0.51661900	0.58829000
H	4.15076600	-0.76003800	-0.44396900
C	3.61339100	0.42239000	1.28087600
C	-1.19643400	2.12061500	-1.60732200
C	1.54540200	-2.22970500	1.27310700
C	2.75666700	-4.25268100	-0.16973400
C	-2.09102300	-3.15354200	0.79952600
C	3.13778600	2.67019800	-0.46422800
C	1.69533300	3.21703500	2.33170500
H	2.69587900	3.58572300	2.12007500
C	2.19524400	-3.30031400	1.95796700
H	2.16571400	-3.31101500	3.04222900
C	-3.61235500	0.42756400	-1.28100000
C	-2.20237800	-3.29530600	-1.95757400
H	-2.17330700	-3.30639100	-3.04184600
C	-1.95783800	-3.19387000	2.20567000
H	-1.41806300	-2.40378000	2.70486900
C	2.81901000	-4.27659800	1.24560700
H	3.32959400	-5.09662700	1.74617900
C	3.90756200	0.70628800	2.62034300
H	3.29259400	1.40342700	3.17998100
C	5.46142300	-1.14129800	1.22561700
H	6.05703000	-1.86704200	0.67798500
C	-2.49491900	3.90779800	0.65898600

H	-1.48170800	4.05755800	0.30077000
C	-0.87012000	2.28446100	2.82058900
H	-1.87170100	1.93526300	3.03577800
C	1.95398800	-3.19844200	-2.20552400
H	1.41802600	-2.40608700	-2.70527000
C	-1.54876300	-2.22663600	-1.27326200
C	-1.69044500	3.21909400	-2.33204000
H	-2.69050000	3.58911900	-2.12042700
C	2.50115000	3.90418900	-0.65930000
H	1.48804900	4.05541200	-0.30138100
C	0.87366900	2.28293300	-2.82098600
H	1.87473400	1.93231900	-3.03624600
C	3.30865500	-5.29491900	-0.94812300
H	3.81921500	-6.10761700	-0.43578500
C	4.97717300	0.07523600	3.24993800
H	5.19385100	0.30065700	4.29107500
C	-3.90550300	0.71118400	-2.62074500
H	-3.28903100	1.40684000	-3.18057500
C	-4.43504900	2.50342400	0.95358300
H	-4.94651800	1.55647000	0.82334700
C	-2.76621000	-4.24525800	0.17062200
C	5.09264400	3.53950400	-1.60579500
H	6.10291700	3.38735000	-1.97630300
C	-0.35959900	3.36110900	3.54688400
H	-0.98636400	3.82564200	4.30448900
C	4.43940600	2.49705200	-0.95315400
H	4.94945300	1.54936300	-0.82266700
C	-4.97609200	0.08177100	-3.25032900
H	-5.19198700	0.30698200	-4.29167500
C	-3.15255100	4.95115300	1.30551800
H	-2.64426800	5.90250800	1.44001400
C	-4.45022100	4.77409800	1.78119400
H	-4.96341000	5.58887600	2.28578200
C	2.48680300	-4.23786600	-2.93912800
H	2.36364800	-4.23542000	-4.01905200
C	-2.82929500	-4.26919600	-1.24470600
H	-3.34299300	-5.08751500	-1.74489100
C	-5.08659600	3.54683500	1.60638800
H	-6.09695500	3.39611200	1.97724600
C	4.45804800	4.76765300	-1.78089500
H	4.97256600	5.58168800	-2.28533200
C	0.92425800	3.83786000	3.30627100
H	1.32317200	4.67908000	3.86716700
C	5.75938800	-0.84581500	2.55384300
H	6.59338800	-1.33686300	3.04920000
C	0.36461300	3.36025800	-3.54731700
H	0.99201400	3.82388400	-4.30495000
C	-0.91857600	3.83879200	-3.30669200
H	-1.31637200	4.68050900	-3.86763500
C	-3.32137800	-5.28541200	0.94953500
H	-3.83522100	-6.09634600	0.43768200
C	-5.46330800	-1.13268300	-1.22547100
H	-6.06042200	-1.85703100	-0.67763700
C	-2.49381800	-4.23131700	2.93977600
H	-2.36948900	-4.22943900	4.01956900
C	3.18356500	-5.29113400	-2.31808400
H	3.60392200	-6.09727200	-2.91339000
C	-5.76029500	-0.83737200	-2.55395700
H	-6.59506500	-1.32711400	-3.04931000
C	-3.19517500	-5.28193200	2.31940200

H	-3.61802000	-6.08645500	2.91513000
C	3.16047300	4.94658000	-1.30566900
H	2.65360300	5.89866000	-1.44037100
Cl	-2.77747200	-0.20664800	2.55876000
Cl	2.77795800	-0.21003300	-2.55871600

3d

Pd	0.77141700	0.49172900	1.04475400
P	2.26795500	-0.85921900	-0.15599000
S	-0.82905500	1.72763900	2.28643100
N	1.53442700	2.41474900	0.22810800
C	-1.58387600	2.73202000	1.09126200
Pd	-0.77138500	0.49173300	-1.04481800
P	-2.26795200	-0.85918800	0.15599000
S	0.82918600	1.72760200	-2.28643700
N	-1.53439200	2.41474000	-0.22810700
C	-2.69566400	4.68827900	0.69475600
H	-3.20014900	5.55848400	1.11377300
C	-2.57619500	4.51367500	-0.68320700
H	-2.94196800	5.24135400	-1.39864700
C	-1.98830100	3.33189000	-1.10036200
H	-1.89033500	3.07344200	-2.14854500
C	1.58391600	2.73203500	-1.09125500
C	2.69558600	4.68835800	-0.69472000
H	3.20003400	5.55858900	-1.11372700
C	2.57611500	4.51373400	0.68323800
H	2.94184600	5.24141900	1.39869400
C	1.98828400	3.33191000	1.10037900
H	1.89034000	3.07343700	2.14856400
C	1.36642400	-1.66303400	-1.50561500
C	0.10106800	-1.17565500	-1.88649700
C	-0.53830500	-1.80419800	-2.96335800
H	-1.50958700	-1.45517600	-3.28964300
C	0.05931500	-2.86698600	-3.63987800
H	-0.46843000	-3.32067300	-4.47558700
C	1.30819500	-3.34701800	-3.25505300
H	1.77352900	-4.17694900	-3.78045500
C	1.95471700	-2.74520100	-2.18414200
H	2.92627600	-3.11186000	-1.86213400
C	3.67888500	0.05537700	-0.89036200
C	4.02162600	-0.09736400	-2.23943500
H	3.42013100	-0.72507400	-2.88835100
C	5.12464700	0.57472500	-2.76085900
H	5.37724000	0.45323300	-3.81087500
C	5.89094600	1.40668500	-1.94703700
H	6.74985600	1.93072100	-2.35858400
C	5.54403600	1.57529000	-0.60776700
H	6.12873200	2.23204500	0.03132000
C	4.43887300	0.91138400	-0.07922200
H	4.15673800	1.06259400	0.96009400
C	3.04350500	-2.23684600	0.78005700
C	4.29850000	-2.09260400	1.38485000
H	4.84782700	-1.16275400	1.29189500
C	4.86002500	-3.14552000	2.10343900
H	5.83609700	-3.01700500	2.56368400
C	4.17844600	-4.35401400	2.22901200
H	4.62132200	-5.17575500	2.78605100
C	2.92622300	-4.50442200	1.63583200
H	2.38409000	-5.44173600	1.72995000

C	2.35820700	-3.45226700	0.92275500
H	1.38031200	-3.58019700	0.46969800
C	-1.36640200	-1.66303900	1.50557400
C	-0.10103200	-1.17567200	1.88643400
C	0.53838400	-1.80427300	2.96323300
H	1.50967600	-1.45526100	3.28949700
C	-0.05920800	-2.86709400	3.63972500
H	0.46858100	-3.32083300	4.47537900
C	-1.30811800	-3.34709000	3.25494500
H	-1.77342100	-4.17706100	3.78031400
C	-1.95468500	-2.74521300	2.18409600
H	-2.92625700	-3.11185800	1.86210700
C	-3.67886100	0.05539100	0.89039900
C	-4.43886800	0.91141500	0.07929200
H	-4.15674200	1.06266400	-0.96001700
C	-5.54400900	1.57531900	0.60788100
H	-6.12871500	2.23209200	-0.03117700
C	-5.89087500	1.40669900	1.94715800
H	-6.74977300	1.93072700	2.35874000
C	-5.12455900	0.57472200	2.76094900
H	-5.37712700	0.45321800	3.81097000
C	-4.02156000	-0.09736600	2.23948600
H	-3.42005700	-0.72510900	2.88836500
C	-3.04357800	-2.23677100	-0.78005600
C	-4.29860000	-2.09247800	-1.38478100
H	-4.84790000	-1.16261700	-1.29176900
C	-4.86019600	-3.14536000	-2.10336200
H	-5.83628700	-3.01680100	-2.56355700
C	-4.17867000	-4.35387600	-2.22898000
H	-4.62159500	-5.17558600	-2.78602300
C	-2.92643100	-4.50434900	-1.63584800
H	-2.38434600	-5.44169100	-1.72998700
C	-2.35834300	-3.45222400	-0.92278100
H	-1.38044000	-3.58020400	-0.46975500
N	2.19217200	3.82926300	-1.56953000
N	-2.19219800	3.82920300	1.56955300
Cl	2.43174400	0.74746300	2.87812400
Cl	-2.43178500	0.74745700	-2.87803400

3e

Pd	-0.75323600	-0.46256900	1.09599500
P	-2.23383300	0.90373300	-0.07948700
S	0.88118300	-1.74227000	2.30269800
N	1.56781700	-2.28555000	-0.29381800
C	1.51369400	-2.66464500	0.98605900
Pd	0.75325600	-0.46272400	-1.09593900
P	2.23407000	0.90337500	0.07953300
S	-0.88128500	-1.74219400	-2.30260000
C	2.10886100	-3.32657600	-1.01115500
H	2.24750600	-3.24732100	-2.07833900
C	2.16326100	-4.66941700	2.33632700
H	1.35382200	-4.38523700	3.01322300
H	3.12206400	-4.46002300	2.82285600
H	2.09441500	-5.73754500	2.11617800
C	-1.51418300	-2.66431300	-0.98595500
C	2.41547800	-4.34056900	-0.15341500
H	2.87493500	-5.30452600	-0.31410600
N	2.02845700	-3.92170300	1.10524700
C	-2.16535500	-4.66846200	-2.33641200

H	-2.09648500	-5.73666600	-2.11661000
H	-1.35634700	-4.38420600	-3.01377900
H	-3.12446700	-4.45881000	-2.82221400
N	-1.56806900	-2.28529400	0.29395900
C	-2.10961500	-3.32610900	1.01122200
H	-2.24812500	-3.24690300	2.07842600
C	-2.41693500	-4.33980600	0.15339200
H	-2.87643500	-5.30374000	0.31408500
N	-2.02963400	-3.92108000	-1.10523200
C	-1.37946400	1.71086500	-1.45940900
C	-0.14710700	1.19953600	-1.91027800
C	0.43418500	1.81373800	-3.02868000
H	1.37900200	1.44431700	-3.40881400
C	-0.18297400	2.88480100	-3.67280700
H	0.30018400	3.32697800	-4.54125000
C	-1.39623300	3.39114200	-3.21239100
H	-1.87595200	4.23026100	-3.70982700
C	-1.98904900	2.80280800	-2.10357900
H	-2.93440500	3.18578400	-1.72712700
C	-3.66865700	-0.00134800	-0.78225000
C	-4.41290100	-0.85859300	0.04131000
H	-4.10265400	-1.02255800	1.07034500
C	-5.53408900	-1.51293900	-0.46419500
H	-6.10541300	-2.17167800	0.18493200
C	-5.91446700	-1.33244400	-1.79336700
H	-6.78935300	-1.84553000	-2.18544500
C	-5.16374100	-0.49931300	-2.62031900
H	-5.44360800	-0.36525900	-3.66212700
C	-4.04293800	0.16174300	-2.12138400
H	-3.45422900	0.79123900	-2.78008600
C	-2.98357800	2.27739000	0.88400200
C	-2.28763900	3.48716500	1.02267200
H	-1.31709900	3.61123000	0.55288600
C	-2.83517300	4.53788700	1.75340000
H	-2.28482700	5.47072500	1.84448500
C	-4.07731900	4.39145100	2.36860600
H	-4.50425200	5.21215600	2.93958100
C	-4.76881900	3.18825300	2.24780100
H	-5.73665800	3.06250500	2.72597300
C	-4.22765500	2.13682200	1.51137400
H	-4.78412200	1.21082500	1.42261600
C	1.37978100	1.71071300	1.45937700
C	0.14735300	1.19958900	1.91028500
C	-0.43382100	1.81389600	3.02868600
H	-1.37866100	1.44458900	3.40886800
C	0.18349000	2.88490700	3.67274900
H	-0.29958100	3.32717500	4.54119500
C	1.39679500	3.39108600	3.21227200
H	1.87660800	4.23018600	3.70964600
C	1.98951400	2.80262000	2.10347900
H	2.93492200	3.18543900	1.72698900
C	2.98407100	2.27683500	-0.88404900
C	2.28834600	3.48668900	-1.02289900
H	1.31780600	3.61098400	-0.55315900
C	2.83608400	4.53724400	-1.75374000
H	2.28588200	5.47015500	-1.84494800
C	4.07822100	4.39053400	-2.36886400
H	4.50532300	5.21109100	-2.93992400
C	4.76953400	3.18723800	-2.24786400
H	5.73737500	3.06129000	-2.72598200

C	4.22817600	2.13598800	-1.51134000
H	4.78447700	1.20991700	-1.42242400
C	3.66873500	-0.00189300	0.78232800
C	4.41272500	-0.85938900	-0.04119800
H	4.10239100	-1.02336600	-1.07020700
C	5.53383200	-1.51388900	0.46429200
H	6.10495700	-2.17284600	-0.18478900
C	5.91437200	-1.33327600	1.79340200
H	6.78918000	-1.84649600	2.18547500
C	5.16391300	-0.49985800	2.62030600
H	5.44393200	-0.36569700	3.66206100
C	4.04318800	0.16134700	2.12139200
H	3.45466700	0.79106300	2.78005300
Cl	-2.35761700	-0.74093300	2.97685500
Cl	2.35755900	-0.74156600	-2.97683900

3f

Pd	-0.83400000	0.11546900	1.01121600
S	0.62121000	-1.21953000	2.36075300
P	-2.08926400	1.59105500	-0.29600900
N	1.48072300	-3.61676000	1.41456000
C	1.17530700	-2.30892700	1.14548500
Pd	0.84918500	-0.06483400	-1.00980500
P	2.37994100	1.12329800	0.29207200
S	-0.85090100	-1.07224500	-2.35675500
N	1.32757300	-2.03056000	-0.15232500
C	1.40162300	-4.27889000	2.69648700
H	0.79025300	-3.67137100	3.36618400
H	2.39757700	-4.40904100	3.13395400
H	0.92832500	-5.25706200	2.57103300
N	-1.71135200	-1.71249600	0.15838400
C	1.82284000	-4.21827600	0.21911800
N	-2.21956700	-3.21895300	-1.41215400
C	2.19779800	-5.52864800	-0.06940800
H	2.30192500	-6.27674900	0.71119800
C	2.42536800	-5.83836500	-1.40623300
H	2.71693000	-6.84959100	-1.67764400
C	2.27747500	-4.86546900	-2.40738800
H	2.45639300	-5.13962000	-3.44391900
C	1.91211500	-3.55577100	-2.11180300
H	1.80845200	-2.80666600	-2.88574200
C	1.69605100	-3.22240900	-0.77117500
C	-1.62795000	-2.01402500	-1.14056400
C	-2.29633200	-3.87623300	-2.69668300
H	-1.55977300	-3.42587300	-3.36463300
H	-3.29489800	-3.76840500	-3.13437900
H	-2.06452200	-4.93817100	-2.57430700
C	-1.01809000	2.30901800	-1.57147400
C	0.21441900	1.69815700	-1.87893400
C	0.97704800	2.26690000	-2.90654100
H	1.92520800	1.81932000	-3.17728100
C	0.53593800	3.39034900	-3.60508500
H	1.15951300	3.79381700	-4.39963500
C	-0.67882600	3.99272000	-3.29141600
H	-1.02368300	4.87104600	-3.83100100
C	-1.44909300	3.45086300	-2.27097800
H	-2.39526100	3.91471200	-2.00375600
C	-2.80867300	3.03309500	0.58583500
C	-4.10868000	2.98483700	1.10534400

H	-4.71382900	2.09416400	0.98016800
C	-4.63764700	4.08080100	1.78265800
H	-5.64857900	4.02721700	2.17784800
C	-3.87807400	5.23660000	1.95169300
H	-4.29517000	6.09237100	2.47660800
C	-2.58097500	5.29055200	1.44464200
H	-1.97835000	6.18576700	1.57444000
C	-2.04575800	4.19475800	0.77288500
H	-1.03289300	4.24672500	0.38702000
C	-3.53042900	0.81588300	-1.13007000
C	-3.82188700	1.08652700	-2.47260800
H	-3.16114200	1.71559000	-3.05993400
C	-4.95131500	0.53032100	-3.06878100
H	-5.16616800	0.74567200	-4.11240900
C	-5.79387900	-0.30440100	-2.33631000
H	-6.67411200	-0.73751800	-2.80518400
C	-5.49987400	-0.58735900	-1.00360300
H	-6.14421500	-1.24601700	-0.42705500
C	-4.37099200	-0.03611100	-0.39980400
H	-4.13516600	-0.27329800	0.63450900
C	1.48334000	2.05067700	1.56655100
C	0.14969000	1.71269500	1.87103400
C	-0.48071400	2.43279100	2.89348300
H	-1.50310800	2.19600200	3.16018500
C	0.18480700	3.44002700	3.59145800
H	-0.34219800	3.96793700	4.38301400
C	1.50024100	3.77235100	3.28124000
H	2.02025300	4.55964400	3.82099400
C	2.14255100	3.07865800	2.26428800
H	3.16540000	3.33332600	1.99849300
C	3.37980300	2.38621900	-0.59033000
C	2.86735700	3.67738600	-0.78156900
H	1.88252600	3.93174800	-0.40352200
C	3.61725100	4.64327700	-1.44714100
H	3.20830700	5.64155700	-1.57992200
C	4.88110600	4.32951400	-1.94376300
H	5.46636200	5.08406000	-2.46338300
C	5.39152700	3.04451200	-1.77081200
H	6.37446400	2.78915700	-2.15768300
C	4.64780800	2.07726600	-1.09912200
H	5.06080900	1.08345600	-0.96755500
C	3.63027100	0.06882500	1.12758300
C	3.96602000	0.27266900	2.47162900
H	3.44518500	1.02225900	3.05815200
C	4.95524500	-0.50334800	3.07105600
H	5.20511300	-0.33775100	4.11595700
C	5.61241100	-1.49183900	2.34015700
H	6.38343700	-2.09661400	2.81133100
C	5.27168300	-1.70742500	1.00592800
H	5.76982100	-2.48357900	0.43068100
C	4.28177400	-0.93656900	0.39889100
H	4.00652700	-1.11902600	-0.63679000
C	-2.33471800	-2.79427300	0.77547200
C	-2.68464400	-3.73267600	-0.21738300
C	-3.34178700	-4.92730400	0.06815400
H	-3.61338200	-5.62942300	-0.71495400
C	-3.62692200	-5.18485700	1.40506600
H	-4.13588800	-6.10664500	1.67428500
C	-3.26090700	-4.27428300	2.40884300
H	-3.49178600	-4.50649700	3.44533700

C	-2.61425700	-3.07732000	2.11589700
H	-2.34325600	-2.37382200	2.89219400
Cl	2.63270200	-0.40997800	-2.71016900
Cl	-2.64560200	0.14595500	2.71350200

3g

Pd	-0.86353800	0.00422700	0.98380300
S	0.70707200	-1.14230100	2.36275400
P	-2.25056300	1.34489700	-0.34357600
C	1.43767800	-2.17351500	1.19920800
Pd	0.86351800	0.00406500	-0.98379400
P	2.25068300	1.34462700	0.34347700
S	-0.70726400	-1.14227100	-2.36278000
N	1.52785900	-1.97136500	-0.10131000
N	-1.52818800	-1.97123100	0.10124600
C	2.50926200	-4.10563800	0.10861400
C	3.10103300	-5.27713100	-0.36085400
H	3.42755700	-6.04941100	0.32964400
C	3.23835400	-5.43636400	-1.73418500
H	3.68966600	-6.34328300	-2.12762100
C	2.77891300	-4.44461500	-2.60993500
H	2.87290500	-4.59044100	-3.68258500
C	2.19960300	-3.27280100	-2.14064300
H	1.84957900	-2.51249800	-2.82469500
C	2.07830900	-3.07871000	-0.75900900
C	-1.43791900	-2.17343900	-1.19924200
C	-1.22846700	2.16965400	-1.59257000
C	0.07045600	1.69619500	-1.86387400
C	0.80186800	2.34463100	-2.86585800
H	1.80049900	2.00392700	-3.10736800
C	0.26392300	3.41662000	-3.57796800
H	0.86545800	3.88552500	-4.35316700
C	-1.01697600	3.88459200	-3.30265800
H	-1.43722600	4.72170100	-3.85394800
C	-1.75529600	3.26163000	-2.30527400
H	-2.75226400	3.62297100	-2.06614700
C	-3.12658100	2.70783700	0.52079800
C	-4.42597900	2.52910800	1.01289500
H	-4.93472200	1.58107600	0.87953900
C	-5.07861200	3.56826500	1.67142700
H	-6.08733600	3.41336700	2.04481400
C	-4.44519400	4.79670600	1.84853600
H	-4.95933100	5.60781300	2.35795500
C	-3.14985700	4.98078000	1.36868000
H	-2.64518700	5.93383100	1.50429400
C	-2.49083500	3.94234300	0.71611000
H	-1.48023700	4.09677000	0.35228200
C	-3.58684900	0.42828900	-1.20628100
C	-3.87829200	0.67254300	-2.55416000
H	-3.27274600	1.36536800	-3.12907400
C	-4.93453700	0.00753700	-3.17187500
H	-5.14853100	0.20078800	-4.21985500
C	-5.70351500	-0.90841700	-2.45583900
H	-6.52454300	-1.42864600	-2.94270400
C	-5.40848400	-1.16407800	-1.11815100
H	-5.99376700	-1.88654100	-0.55549600
C	-4.35158300	-0.50524400	-0.49245900
H	-4.11326200	-0.71911200	0.54630500
C	1.22869800	2.16954900	1.59246400

C	-0.07030100	1.69631800	1.86380400
C	-0.80168000	2.34500000	2.86564200
H	-1.80039700	2.00452300	3.10710100
C	-0.26359100	3.41697900	3.57766900
H	-0.86510100	3.88607700	4.35277100
C	1.01741300	3.88467100	3.30240200
H	1.43778200	4.72177100	3.85361600
C	1.75567200	3.26149200	2.30510500
H	2.75271000	3.62264000	2.06601600
C	3.12691400	2.70746800	-0.52082300
C	2.49116300	3.94192800	-0.71642200
H	1.48046600	4.09635700	-0.35286400
C	3.15031600	4.98032700	-1.36892100
H	2.64564500	5.93334600	-1.50476900
C	4.44578500	4.79625000	-1.84841500
H	4.96003000	5.60731900	-2.35778300
C	5.07920500	3.56784900	-1.67102700
H	6.08803700	3.41296400	-2.04412700
C	4.42643800	2.52872500	-1.01257900
H	4.93515000	1.58070100	-0.87899700
C	3.58680100	0.42785000	1.20632700
C	3.87807000	0.67205200	2.55425700
H	3.27247800	1.36492000	3.12908300
C	4.93416200	0.00694800	3.17212100
H	5.14804400	0.20016400	4.22012900
C	5.70316200	-0.90905800	2.45617400
H	6.52406700	-1.42938000	2.94315200
C	5.40829400	-1.16468600	1.11844800
H	5.99360400	-1.88719300	0.55588000
C	4.35154100	-0.50575700	0.49260400
H	4.11332600	-0.71959300	-0.54618600
C	-2.07867800	-3.07856300	0.75896400
C	-2.50966100	-4.10549200	-0.10864800
C	-3.10154700	-5.27693000	0.36080600
H	-3.42810300	-6.04918300	-0.32970600
C	-3.23895200	-5.43613400	1.73413400
H	-3.69037800	-6.34300000	2.12756400
C	-2.77943700	-4.44441700	2.60988000
H	-2.87345300	-4.59021900	3.68253200
C	-2.20001500	-3.27265700	2.14058900
H	-1.84986800	-2.51243400	2.82465800
S	-2.11998300	-3.69089100	-1.75450600
S	2.11971100	-3.69092000	1.75445800
Cl	2.71601100	-0.13909500	-2.63329300
Cl	-2.71559200	-0.13889900	2.63344000

3h

Pd	0.75054200	-0.45890200	-1.10120500
S	-0.83964200	-1.77241900	-2.34928100
P	2.22731400	0.90473700	0.06815800
N	1.55388500	-2.28372400	-0.25343000
C	-1.51238800	-2.63902100	-1.03718200
Pd	-0.75051000	-0.45866800	1.10123500
P	-2.22704000	0.90519000	-0.06817000
S	0.83955500	-1.77240700	2.34929400
N	-1.55424600	-2.28335500	0.25344600
C	1.51171300	-2.63944700	1.03717100
N	2.13508200	-3.28335100	-0.94584500
C	2.29939400	-4.70614200	2.24535700

H	1.37982000	-4.74134800	2.83546300
H	3.11443000	-4.31995200	2.86419600
H	2.55169200	-5.70072100	1.87677300
N	2.47362800	-4.22771400	-0.15059800
C	-2.30164800	-4.70503000	-2.24548800
H	-1.38230600	-4.74060400	-2.83592800
H	-3.11669800	-4.31825000	-2.86394200
H	-2.55433500	-5.69955600	-1.87703300
N	2.09190900	-3.85560200	1.09587500
N	-2.13615300	-3.28259300	0.94581900
N	-2.47524500	-4.22674800	0.15056000
N	-2.09329100	-3.85483800	-1.09591100
C	1.37563300	1.71559900	1.44605300
C	0.15055800	1.20013600	1.91139700
C	-0.42449500	1.80943300	3.03449400
H	-1.36331500	1.43321800	3.42292400
C	0.19397700	2.88439800	3.67106600
H	-0.28256300	3.32374300	4.54439700
C	1.39938500	3.39727000	3.19780000
H	1.87905400	4.23954800	3.68963200
C	1.98511700	2.81148900	2.08396700
H	2.92470700	3.19892700	1.69812000
C	3.64608000	-0.02095900	0.77505700
C	4.02598800	0.15510300	2.11152700
H	3.45286600	0.80667700	2.76254200
C	5.13369500	-0.52186000	2.61813500
H	5.41872000	-0.37763000	3.65709900
C	5.86413500	-1.38401500	1.80260900
H	6.72747700	-1.91100400	2.20140800
C	5.47806500	-1.57650500	0.47665000
H	6.03134600	-2.25884100	-0.16316800
C	4.37152200	-0.90472200	-0.03846700
H	4.05766600	-1.07911000	-1.06508800
C	2.98466900	2.26423800	-0.90316800
C	4.22526800	2.10254000	-1.53257400
H	4.76649200	1.16754600	-1.44428600
C	4.77911000	3.14433800	-2.27277700
H	5.74345400	3.00371100	-2.75352200
C	4.10360600	4.35658200	-2.39531400
H	4.54066900	5.16940200	-2.96974100
C	2.86472300	4.52284400	-1.77846400
H	2.32780000	5.46321100	-1.87140500
C	2.30392800	3.48232500	-1.04320700
H	1.33610400	3.62131100	-0.57185000
C	-1.37526400	1.71575200	-1.44616800
C	-0.15028700	1.19999600	-1.91144900
C	0.42487100	1.80906100	-3.03462400
H	1.36361600	1.43262800	-3.42302700
C	-0.19339600	2.88407900	-3.67131000
H	0.28323800	3.32324200	-4.54468100
C	-1.39870100	3.39723600	-3.19809400
H	-1.87821900	4.23955100	-3.69000900
C	-1.98453700	2.81169100	-2.08419200
H	-2.92404200	3.19936400	-1.69837800
C	-2.98412300	2.26491900	0.90303400
C	-4.22469800	2.10355100	1.53256000
H	-4.76611100	1.16864700	1.44445900
C	-4.77829800	3.14557000	2.27264100
H	-5.74263300	3.00518800	2.75347600
C	-4.10257300	4.35771200	2.39492600

H	-4.53944900	5.17070300	2.96925300
C	-2.86370600	4.52365500	1.77794900
H	-2.32660900	5.46394200	1.87069800
C	-2.30315100	3.48291800	1.04282500
H	-1.33533900	3.62165200	0.57137400
C	-3.64601600	-0.02034600	-0.77487000
C	-4.02592300	0.15542300	-2.11137700
H	-3.45270100	0.80671900	-2.76257600
C	-5.13377300	-0.52147500	-2.61775900
H	-5.41881200	-0.37747800	-3.65675100
C	-5.86435600	-1.38326900	-1.80197500
H	-6.72780800	-1.91019800	-2.20061600
C	-5.47827800	-1.57548400	-0.47597800
H	-6.03165300	-2.25755100	0.16404500
C	-4.37158700	-0.90376700	0.03891200
H	-4.05769700	-1.07798900	1.06555300
Cl	-2.36143300	-0.71737900	2.94646100
Cl	2.36158200	-0.71800500	-2.94636800