Electronic Supplementary Information

For

Reactivity of bis[{2,6-(dimethylamino)methyl}phenyl]telluride with Pd(II) and Hg(II): Isolation of the first Pd(II) complex of an organotellurenium cation as a ligand

Anand K. Gupta,[a] Rajesh Deka,[a] Harkesh B. Singh[a]* and Ray J. Butcher[b]

[a]Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India

[b]Department of Chemistry, Howard University, Washington DC 20059, USA

E-mail: chhbsia@chem.iitb.ac.in

Contents **Page No.**

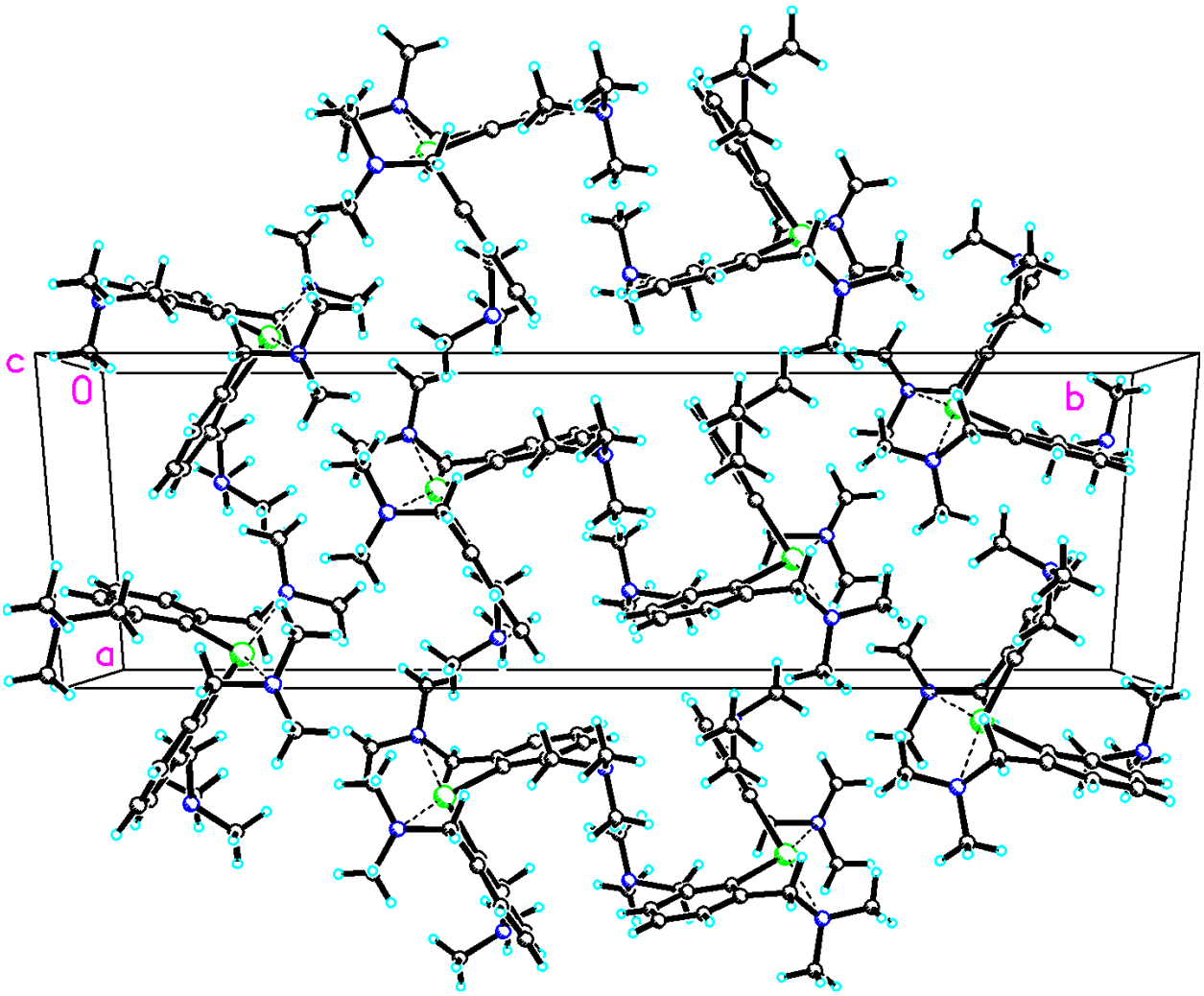


Fig. S1 Packing diagram of compound **6**.

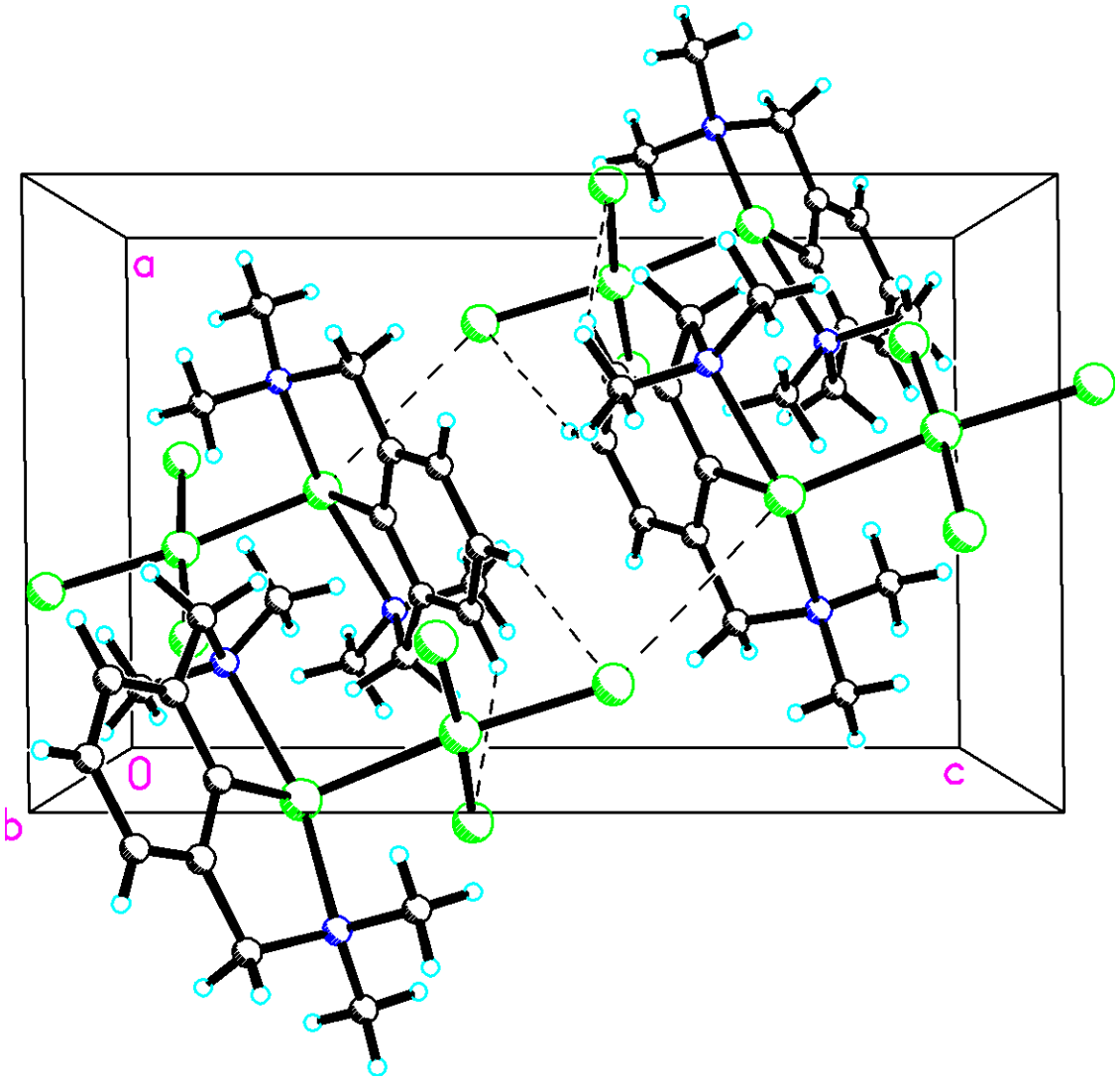


Fig. S2 Packing diagram of complex **7**.

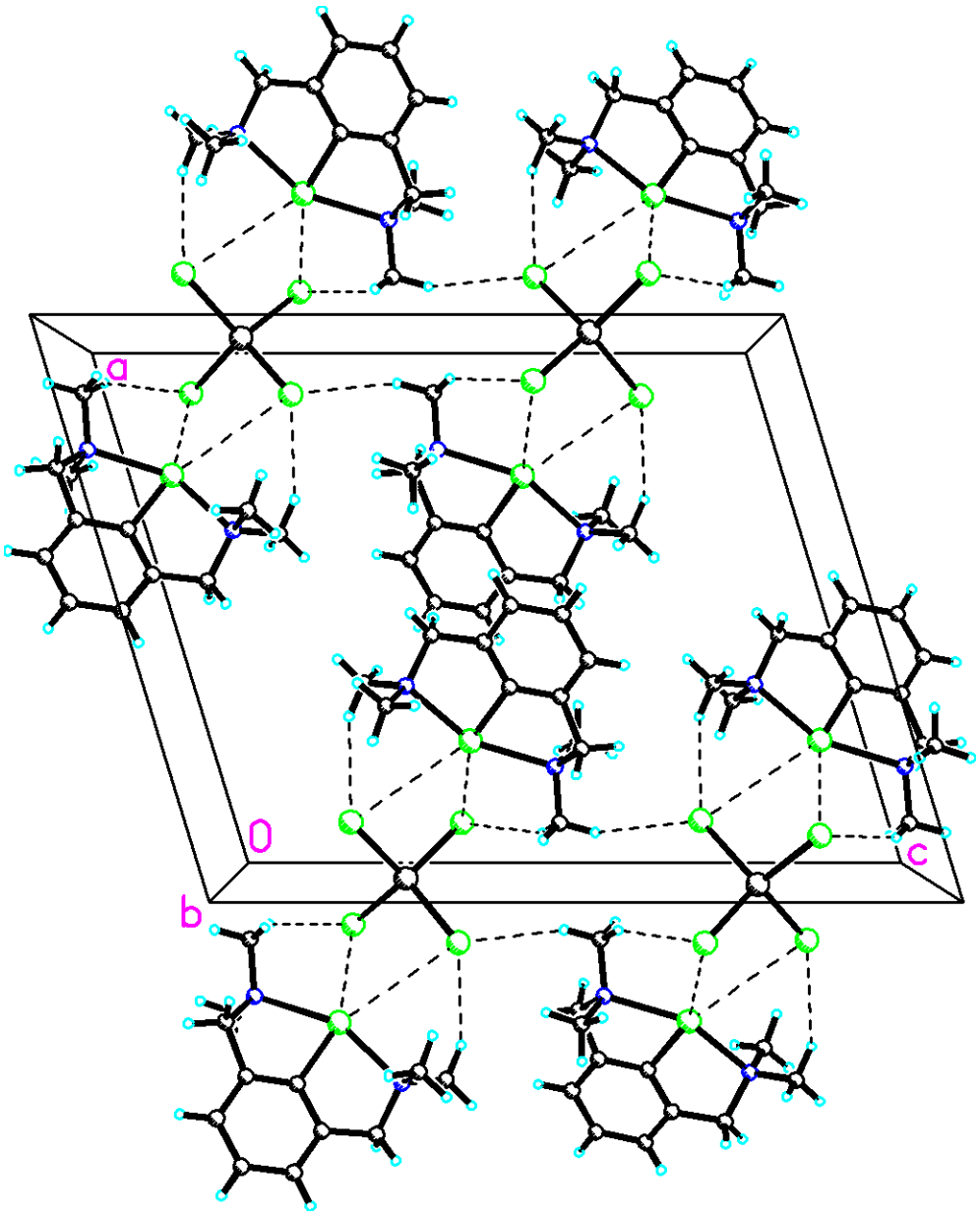


Fig. S3 Packing diagram of **8**.

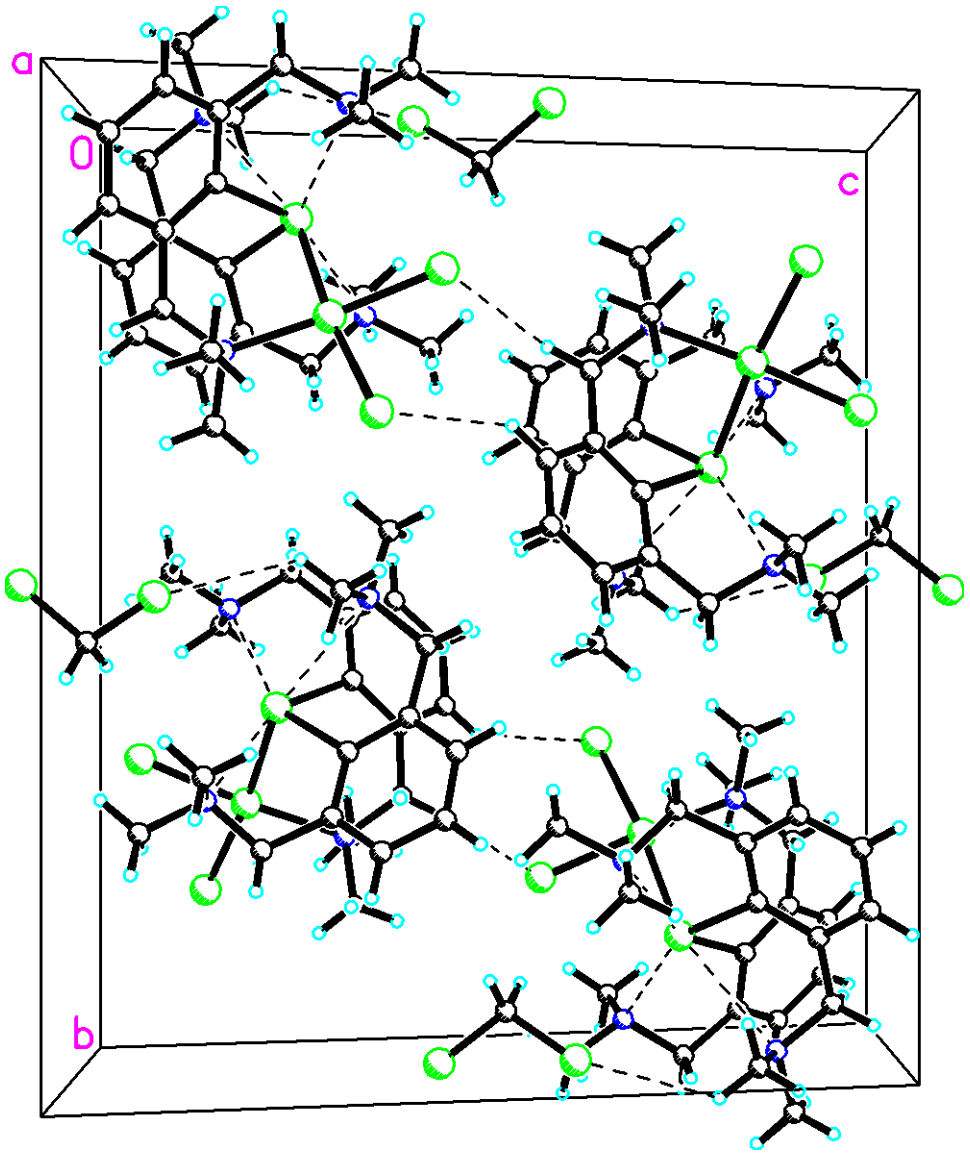


Fig. S4 Packing diagram of complex **9**.

Table S1 Crystallographic Data and Refinement Details for **6-9**.

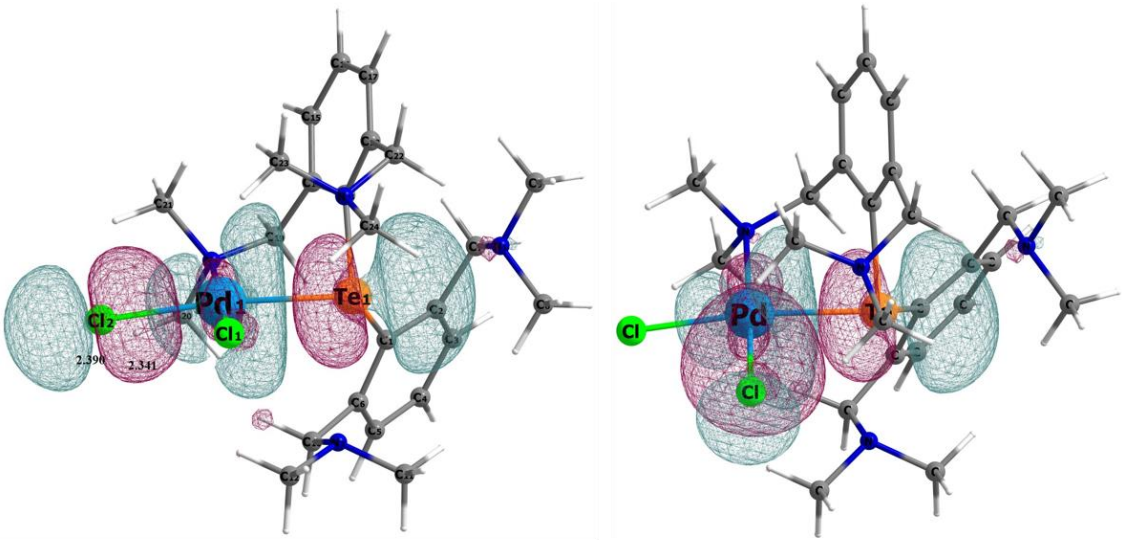
Compound	**6**	**7**	**8**	**9**
Empirical formula	$C_{24}H_{38}N_4Te$	$C_{12}H_{19}Cl_3N_2PdTe$	$C_{24}H_{38}Cl_4HgN_4Te_2$	$C_{49}H_{78}Cl_6N_8Pd_2Te_2$
F. W. (g/mol)	510.18	531.64	980.17	1459.89
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$C2/c$	$P2_1/c$
a (Å)	9.39820(17)	8.8060(18)	15.052(4)	9.3657(2)
b (Å)	29.1571(4)	13.281(3)	12.069(3)	18.9012(3)
c (Å)	10.11713(16)	14.315(3)	18.453(4)	16.6559(3)
α (°)	90	90	90	90
β (°)	114.042(2)	90.64(3)	106.982(3)	103.849(2)
γ (°)	90	90	90	90
V (Å^3)	2531.83(8)	1674.1(6)	3206.1(14)	2862.76(10)
Z	4	4	4	2
D(calcd) (Mg/m^3)	1.338	2.109	2.031	1.694
F(000)	1048.0	1016.0	1848.0	1452.0
Range of 2θ(deg)	6.062 to 150.938	6.262 to 50.752	6.172 to 58.254	4.31 to 62.346
Collected reflections	9872	12723	4279	29902
Final R_1 [I > 2σ(I)]	0.0294	0.0174	0.0349	0.0202
wR2 =	0.0706	0.0401	0.0709	0.0454
R (all data) R1	0.0346	0.0211	0.0470	0.0231
wR2	0.0748	0.0409	0.0811	0.0465
Goodness of fit F^2	1.047	1.012	0.919	1.034

Table S2 Bond lengths (Å) and bond angle (°) comparison of crystal data and Optimized geometry for **6**-**9**.

	6			**7**		
		Exp.	**Calc.**		**Exp.**	**Calc.**
(Å)	C1A−Te	2.140(2)	2.186	C1−Te1	2.075(2)	2.099
	C1B−Te	2.086(5)	2.179	N2-Te1	2.355(2)	2.416
	N2A−Te	3.192(3)	3.125	N1−Te1	2.337(2)	2.396
	N1B−Te	2.975(3)	3.083	Te1−Pd1	2.5079(8)	2.572
(°)				Pd1−Cl1	2.3129(7)	2.366
				Pd1−Cl2	2.994(7)	2.407
				Pd1-Cl3	2.3535(9)	2.440
	C1A−Te−C1B	99.0(2)	97.84	C1−Te1−Pd1	114.59(6)	114.89
				C1- Te1−N2	76.00(7)	75.57
				C1-Te1-N1	76.22(8)	76.03
				Te1−Pd1−Cl3	172.48(2)	173.06

Table S3 Bond lengths (Å) and bond angle (°) comparison of crystal data and Optimized geometry for **8**-**9**.

	8			**9**		
		Exp.	**Calc.**		**Exp.**	**Calc.**
(Å)	C1−Te1	2.075(4)	2.107	C1A−Te1	2.171(1)	2.210
	N1−Te1	2.342(4)	2.441	C1−Te1	2.142(2)	2.182
	N2−Te1	2.347(5)	2.417	N3−Te1	3.018(1)	3.007
	Hg−Cl1	2.5113(12)	2.621	N4−Te1	3.145(1)	3.445
	Hg−Cl2	2.4686(13)	2.674	N2−Te1	2.942(1)	2.932
				N1−Pd	2.127(1)	2.214
				Te1−Pd	2.5528(4)	2.671
				Pd−Cl1	2.3883(5)	2.408
				Pd−Cl1A	2.3156(5)	2.364
(°)	C1−Te1−N1	75.9(2)	74.76	C1A−Te−Cl	95.08(6)	96.17
	C1−Te1−N2	75.7(2)	75.48	N1−Pd−Te1	96.59(4)	96.53
	Cl1−Hg−Cl2	108.83(4)	106.92			



a) b)

Fig. S5 NBO plot of complex **9** showing a) σ(Cl)→σ*(Te-Pd) and b) σ(Cl)→σ*(Te-Pd) (isosurface value 0.03).

Table S4 Summary of the NPA and NBO on the **6-9** at B3LYP* level of theory.

Comp.		q_N	q_M	$r_{Y\cdots M}$(Å)	χ	$E_{Y\cdots M}$(kj/mole)	E_{el}
6	N2-Te1	-0.558	0.661 (Te)	3.08	0.35	04.58	39.69
	N3-Te1	-0.557		3.12	0.32	04.02	39.18
7	N1-Te	-0.551	1.180 (Te)	2.35	0.80	70.38	88.82
	N2-Te	-0.555		2.37	0.78	65.28	89.83
8	Te-1Hg1		1.190 (Te)	4.15	-0.08	06.49	89.43
	N1-Te6	-0.552	0.940 (Hg)	2.42	0.78	65.79	71.28
	N2-Te6	-0.554		2.44	0.78	61.00	70.83
9	N1-Pd	-0.493	0.120 (Pd)	2.21	0.91	27.14	08.87
	N2-Te	-0.562	1.127 (Te)	2.93	0.45	09.38	71.71
	N3-Te	-0.558		3.01	0.40	08.61	69.44
	N4-Te	-0.560		3.44	0.11	01.76	60.83

Table S5 Cartesian coordinates for compound **6-9**.

Compound 6

Te	0.127082000	1.256449000	-0.196147000
N	-0.498919000	-1.969243000	3.355548000
N	-2.551204000	2.705360000	-0.682414000
C	-1.570700000	-0.012724000	0.308681000
C	-1.500640000	-1.044588000	1.264346000
C	-2.637099000	-1.830058000	1.498167000
H	-2.558604000	-2.625786000	2.230375000
C	-3.834078000	-1.581648000	0.841718000
H	-4.704398000	-2.199430000	1.040440000
C	-3.916968000	-0.518558000	-0.051784000
H	-4.859750000	-0.291794000	-0.542019000
C	-2.799360000	0.270029000	-0.325957000
C	-0.236521000	-1.366306000	2.048365000
H	0.372626000	-2.069066000	1.472508000
H	0.374433000	-0.454149000	2.145594000
C	0.669255000	-2.668272000	3.870493000
H	0.981637000	-3.444828000	3.168676000
H	0.419849000	-3.151450000	4.818694000
H	1.534002000	-2.001735000	4.048208000
C	-0.992257000	-0.991117000	4.316398000
H	-1.888313000	-0.503371000	3.929479000
H	-0.247488000	-0.205968000	4.544280000
H	-1.256656000	-1.490024000	5.252138000
C	-2.931351000	1.426516000	-1.292615000
H	-2.263189000	1.267560000	-2.145789000
H	-3.960398000	1.462077000	-1.691974000
C	-3.476640000	3.121168000	0.364539000
H	-3.103378000	4.028854000	0.843957000
H	-3.556515000	2.342779000	1.124118000
H	-4.490660000	3.329386000	-0.022874000
C	-2.369231000	3.746337000	-1.683756000
H	-2.038574000	4.668767000	-1.200739000
H	-3.294122000	3.968863000	-2.245453000
H	-1.597615000	3.441698000	-2.394414000
N	3.036936000	2.310900000	0.237101000
N	-0.021649000	-2.931979000	-2.723634000
C	1.612161000	-0.325355000	-0.464981000
C	2.856869000	-0.154967000	0.175418000
C	3.857184000	-1.116238000	0.013542000
H	4.811102000	-0.977723000	0.514937000
C	3.647096000	-2.231057000	-0.788615000
H	4.429241000	-2.974072000	-0.910908000
C	2.441332000	-2.369496000	-1.463071000

H	2.271706000	-3.203708000	-2.134012000
C	1.415749000	-1.427105000	-1.321950000
C	3.151140000	1.070376000	1.013090000
H	4.151883000	0.974941000	1.470711000
H	2.431093000	1.138373000	1.835194000
C	3.022994000	3.482313000	1.101578000
H	2.886340000	4.383740000	0.499529000
H	3.956308000	3.599266000	1.681508000
H	2.188326000	3.414090000	1.802835000
C	4.060770000	2.421001000	-0.794853000
H	3.879103000	3.314930000	-1.395817000
H	4.023626000	1.553804000	-1.454759000
H	5.081383000	2.490258000	-0.375636000
C	0.168882000	-1.583704000	-2.186009000
H	-0.722429000	-1.252108000	-1.638886000
H	0.274840000	-0.896090000	-3.033320000
C	-0.844689000	-2.924189000	-3.923947000
H	-0.922424000	-3.939400000	-4.321579000
H	-0.382172000	-2.298894000	-4.691409000
H	-1.871386000	-2.551497000	-3.749541000
C	-0.563205000	-3.843664000	-1.721850000
H	0.089159000	-3.869378000	-0.847056000
H	-0.613292000	-4.855571000	-2.132162000
H	-1.573891000	-3.556123000	-1.383084000

Compound 7

Te	0.353423000	0.238741000	-0.979114000
Pd	-1.836229000	-0.257081000	0.357351000
Cl	-0.706172000	-1.415793000	2.153182000
Cl	-2.688262000	1.075414000	-1.521614000
Cl	-3.967208000	-0.549981000	1.360912000
N	0.583542000	2.447320000	-0.015699000
N	1.120246000	-2.073756000	-1.217388000
C	2.106851000	0.124798000	0.189589000
C	2.652978000	-1.121310000	0.476284000
C	3.835963000	-1.170519000	1.214480000
H	4.285494000	-2.128100000	1.459558000
C	4.429561000	0.010366000	1.661686000
H	5.340007000	-0.036771000	2.249323000
C	3.863671000	1.250799000	1.365104000
H	4.337791000	2.162148000	1.717380000
C	2.693760000	1.313161000	0.608062000

C	2.054236000	2.607565000	0.157341000
H	2.253834000	3.425039000	0.858795000
H	2.466464000	2.903358000	-0.812763000
C	-0.107342000	2.479301000	1.301872000
H	0.061997000	3.451843000	1.777246000
H	0.270115000	1.684200000	1.942441000
H	-1.174132000	2.326617000	1.152686000
C	0.018233000	3.479225000	-0.917430000
H	0.165048000	4.475972000	-0.488038000
H	-1.045004000	3.287668000	-1.052501000
H	0.510802000	3.428467000	-1.888823000
C	1.893027000	-2.346950000	0.030320000
H	2.557601000	-3.203440000	-0.133195000
H	1.170985000	-2.606368000	0.808048000
C	-0.029591000	-3.000580000	-1.352378000
H	0.325231000	-4.035396000	-1.411168000
H	-0.583617000	-2.764712000	-2.261475000
H	-0.690658000	-2.889194000	-0.494405000
C	1.992310000	-2.139336000	-2.410353000
H	2.375453000	-3.156730000	-2.546947000
H	2.834959000	-1.458179000	-2.291934000
H	1.425627000	-1.853186000	-3.296464000

Compound 8

Hg	-0.000015000	-1.716178000	-0.000344000
Cl	-2.244988000	-3.031049000	-0.322290000
Cl	-0.323829000	-0.133310000	2.130687000
Cl	2.244999000	-3.031143000	0.320919000
Cl	0.323706000	-0.132246000	-2.130588000
Te	-3.781148000	-0.024500000	0.295273000
N	-4.439171000	-0.362793000	-2.005535000
N	-4.000032000	1.181094000	2.406250000
C	-7.317171000	3.243465000	-0.473969000
H	-8.107739000	3.966060000	-0.645999000
C	-6.735740000	2.580220000	-1.556425000
H	-7.074207000	2.793002000	-2.566789000
C	-5.709328000	1.660900000	-1.339787000
C	-5.298946000	1.399745000	-0.035150000
C	-5.881764000	2.042427000	1.055724000
C	-6.888100000	2.981098000	0.828857000
H	-7.350120000	3.498954000	1.664981000
C	-5.423123000	1.608880000	2.428557000
H	-5.565974000	2.396084000	3.179370000
H	-6.011386000	0.741083000	2.745433000
C	-3.084920000	2.347191000	2.387590000

H	-2.061247000	1.992125000	2.277666000
H	-3.181871000	2.914078000	3.322053000
H	-3.336786000	2.996541000	1.549368000
C	-3.677074000	0.291118000	3.545001000
H	-4.317289000	-0.590401000	3.510329000
H	-3.832768000	0.816798000	4.494903000
H	-2.636029000	-0.021480000	3.467652000
C	-4.944872000	0.968647000	-2.442527000
H	-5.545935000	0.851988000	-3.352348000
H	-4.066100000	1.567183000	-2.702766000
C	-5.513313000	-1.383129000	-2.032710000
H	-5.121378000	-2.317210000	-1.633293000
H	-5.855985000	-1.542541000	-3.062174000
H	-6.353269000	-1.052144000	-1.422253000
C	-3.299995000	-0.794011000	-2.857186000
H	-2.466968000	-0.100543000	-2.752939000
H	-3.620897000	-0.838251000	-3.904680000
H	-2.961716000	-1.775351000	-2.532608000
Te	3.781173000	-0.024386000	-0.295285000
N	4.439282000	-0.363690000	2.005344000
N	3.999927000	1.182182000	-2.405712000
C	7.317235000	3.243238000	0.475243000
H	8.107816000	3.965752000	0.647555000
C	6.735845000	2.579524000	1.557433000
H	7.074358000	2.791860000	2.567876000
C	5.709423000	1.660297000	1.340435000
C	5.298982000	1.399720000	0.035702000
C	5.881749000	2.042885000	-1.054914000
C	6.888103000	2.981447000	-0.827679000
H	7.350085000	3.499673000	-1.663596000
C	5.423020000	1.609972000	-2.427916000
H	5.565821000	2.397530000	-3.178368000
H	6.011263000	0.742325000	-2.745240000
C	3.084838000	2.348283000	-2.386427000
H	2.061163000	1.993188000	-2.276614000
H	3.181746000	2.915631000	-3.320615000
H	3.336769000	2.997210000	-1.547898000
C	3.676881000	0.292748000	-3.544862000
H	4.317077000	-0.588802000	-3.510645000
H	3.832535000	0.818871000	-4.494526000
H	2.635834000	-0.019864000	-3.467607000
C	4.945010000	0.967558000	2.442901000
H	5.546109000	0.850497000	3.352646000
H	4.066250000	1.565983000	2.703432000
C	5.513417000	-1.384043000	2.032044000
H	5.121473000	-2.317945000	1.632215000

H	5.856105000	-1.543918000	3.061431000
H	6.353365000	-1.052786000	1.421722000
C	3.300123000	-0.795275000	2.856835000
H	2.467100000	-0.101753000	2.752914000
H	3.621050000	-0.839977000	3.904301000
H	2.961824000	-1.776469000	2.531834000

Compound 9

Pd	-2.127779000	0.067818000	0.130407000
Te	0.398713000	0.053929000	-0.737606000
Cl	-4.470734000	0.246747000	0.658873000
N	-1.654670000	-0.118698000	2.285021000
C	1.464627000	1.544743000	0.497999000
C	0.717679000	-1.635187000	0.605802000
Cl	-2.688382000	-0.038394000	-2.163725000
N	0.105143000	-2.498974000	-2.150449000
C	0.406713000	-1.564509000	1.973895000
C	0.895512000	2.832151000	0.583432000
N	-0.180929000	2.863603000	-1.637973000
C	0.650120000	-2.684188000	2.779550000
H	0.430917000	-2.629749000	3.841789000
C	1.499653000	3.805551000	1.384255000
H	1.049875000	4.791976000	1.445360000
N	3.803347000	-0.362355000	-0.420969000
C	1.141970000	-3.865908000	2.238758000
H	1.319286000	-4.725801000	2.876156000
C	2.672473000	3.533923000	2.074646000
H	3.132714000	4.292637000	2.699098000
C	3.281409000	2.297938000	1.908253000
H	4.235308000	2.102960000	2.389105000
C	1.356592000	-3.952114000	0.867230000
H	1.680905000	-4.890593000	0.426817000
C	2.709517000	1.294389000	1.115149000
C	1.141378000	-2.848545000	0.039136000
C	-0.322806000	3.225667000	-0.224532000
H	-1.218275000	2.713051000	0.144974000
H	-0.503049000	4.307428000	-0.102860000
C	-0.206233000	-0.338008000	2.610846000
H	-0.125959000	-0.425920000	3.701946000
H	0.322425000	0.567509000	2.326368000
C	3.513152000	0.013285000	0.966185000
H	4.451659000	0.138426000	1.535910000
H	2.986967000	-0.825364000	1.426004000
C	1.304027000	-2.976671000	-1.461829000
H	2.142152000	-2.356111000	-1.793969000

H	1.549768000	-4.019467000	-1.726410000
C	-2.452151000	-1.257904000	2.811482000
H	-2.165452000	-2.174732000	2.300783000
H	-3.505444000	-1.068776000	2.630318000
H	-2.268959000	-1.373729000	3.888336000
C	0.951443000	3.530573000	-2.279248000
H	1.030804000	3.187807000	-3.312600000
H	1.883763000	3.291546000	-1.766725000
H	0.837154000	4.628200000	-2.289858000
C	-2.086720000	1.129628000	2.962858000
H	-3.132642000	1.314153000	2.731258000
H	-1.484871000	1.964746000	2.605221000
H	-1.956255000	1.038136000	4.049430000
C	-1.417674000	3.156507000	-2.367852000
H	-1.622973000	4.240415000	-2.391882000
H	-2.259067000	2.641889000	-1.909622000
H	-1.333091000	2.795868000	-3.393521000
C	4.534035000	0.675104000	-1.142492000
H	5.520547000	0.890198000	-0.693213000
H	3.961337000	1.602465000	-1.161842000
H	4.694364000	0.354992000	-2.174279000
C	-1.061975000	-3.352112000	-1.931463000
H	-1.942566000	-2.871463000	-2.355844000
H	-1.236950000	-3.481104000	-0.862975000
H	-0.935423000	-4.349753000	-2.386462000
C	4.543982000	-1.618715000	-0.451647000
H	4.706869000	-1.929552000	-1.486302000
H	3.979206000	-2.401386000	0.057705000
H	5.532824000	-1.539583000	0.035851000
C	0.332468000	-2.260739000	-3.570799000
H	0.582571000	-3.184124000	-4.120139000
H	1.151309000	-1.548971000	-3.702018000
H	-0.567394000	-1.828326000	-4.009685000