Electronic Supplementary Information for Dalton Transactions

Innocence and Noninnocence of the ligands in bis(pyrazine-2,3-dithiolate and –diselonate) d^8–metal complexes. A theoretical and experimental study for the Cu(III), Au(III) and Ni(II) cases.

Giuseppe Bruno, Manuel Almeida, Flavia Artizzu, João C. Dias, Maria Laura Mercuri, Luca Pilia, Concepció Rovira, Xavi Ribas, Angela Serpe and Paola Deplano

Supporting Information

Table S1. Selected bond distances (Å) and angles (°) in the optimized $[M(pdt/s)_2]^z$ (M= Cu, Ni, Au; z =0, 1– or 2–) complexes

Compounds	**M-X**	**X-C**	**C1-C2**	**C1/2-N**	**C3/4-N**	**C3-C4**	**X-M-X**	**
$[Ni(pdt)]^{1-}$ $[Ni(pdt)]^{2-}$	2.2008 2.2396	1.7469 1.7462	1.4326 1.4522	1.3389 1.3393	1.3392 1.3495	1.3958 1.3859	92.00 90.53	B
$[Ni(pdt)]^{1-}$ $[Ni(pdt)]^{2-}$	2.1928 2.2288	1.7386 1.7383	1.4262 1.4464	1.3332 1.3324	1.3332 1.3439	1.3884 1.3779	91.78 90.32	BB
$[Ni(pds)]^{1-}$ $[Ni(pds)]^{2-}$	2.3003 2.3296	1.8786 1.8782	1.4250 1.4417	1.3365 1.3383	1.3391 1.3468	1.3954 1.3877	92.17 90.81	B
$[Cu(pdt)]^{0}$ $[Cu(pdt)]^{1-}$	2.2210 2.2377	1.7433 1.7594	1.4257 1.4293	1.3393 1.3308	1.3313 1.3463	1.4075 1.3884	92.96 91.56	B
$[Cu(pdt)]^{1-}$	2.2287	1.7512	1.4229	1.3242	1.3408	1.3803	91.32	BB
$[Cu(pdt)]^{0}$ $[Cu(pdt)]^{1-}$	2.2303 2.2433	1.7776 1.7895	1.4220 1.4271	1.3493 1.3420	1.3444 1.3584	1.4139 1.3963	93.77 92.26	PS
$[Cu(pds)]^{1-}$	2.3329	1.8868	1.4224	1.3308	1.3441	1.3897	91.64	B
$[Cu(pds)]^{1-}$	2.3577	1.9023	1.4195	1.3233	1.3398	1.3812	91.56	BB
$[Cu(pds)]^{0}$ $[Cu(pds)]^{1-}$	2.3365 2.3519	1.9022 1.9139	1.4225 1.4293	1.3511 1.3449	1.3456 1.3579	1.4121 1.3974	94.55 92.74	PS
$[Au(pdt)]^{1-}$	2.4330	1.8094	1.4365	1.3500	1.3612	1.4019	89.20	BS
$[Au(pds)]^{1-}$	2.5384	1.9318	1.4375	1.3533	1.3611	1.4029	89.99	BS
$[Au(pds)]^{1-}$	2.5689	1.9374	1.4366	1.3540	1.3601	1.4022	89.53	BL

** Type of Calculations: B = B3LYP/6-31+G(d,p); BS= B3LYP/SDD; BB = B3LYP/6-311++G(2df,2p); BL = B3LYP/ LANL2DZ; PS = PBE1PBE/SDD

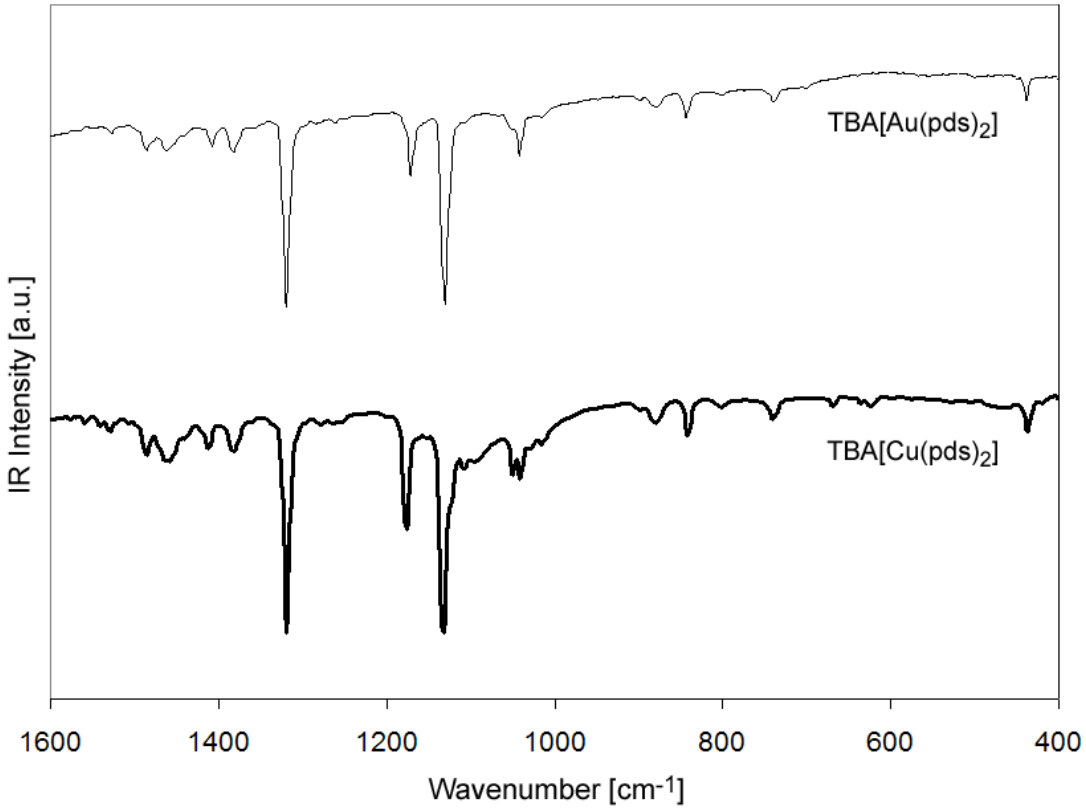


Figure S1. Infrared spectra of TBA[M(pds)$_2$] (M = Cu and Au)

Table S2. Calculated frequencies of the most significant vibrational modes of $[Cu(pdt)_2]^-$ anion.

ν n°	cm^{-1}	$I_{ir.}$	I_{Ra}	Symm.	Mode Assignment
7	148	0	72	Ag	δ(SMS)
11	252	0	9	B2g	butterfly wag
14	333	0	35	Ag	ν(4MS) sy
15	361	36	0	B3u	ν(2MS) asy
20	461	22	0	B1u	rings(6) wag
31	811	0	55	B1g	δ(CCN) +ν(C-S)
32	838	0	12	B2g	H wag
33	839	49	0	B1u	H wag
37	1076	71	0	B3u	ν(CC+CN)+ δ(HCC) + ν(C-S)
38	1077	0	212	Ag	ν(CC+CN)+ δ(HCC) +ν(C-S)
40	1188	752	0	B3u	ν(CC+CN)+ δ(HCC) +ν(C-S)
41	1195	0	148	Ag	ν(CC+CN)+ δ(HCC) +ν(C-S)
44	1272	37	0	B3u	ν(CC+CN)+ δ(HCC)
45	1274	0	151	Ag	ν(CC+CN)+ δ(HCC)
46	1352	478	0	B3u	ν(CC+CN)+ δ(HCC)
48	1451	0	12	B1g	ν(CC+CN)+ δ(HCC)

50	1522	0	337	B1g	v(CN)+ δ(HCC)
51	1523	22	0	B2u	v(CN)+ δ(HCC)
53	1573	0	186	Ag	v(CC+CN)+ δ(HCC)
55	3156	0	284	B1g	v2(CH)sym
56	3176	271	0	B3u	v2(CH)asym
57	3177	0	1429	Ag	v4(CH)sym

Table S3. Calculated frequencies of the most significant vibrational modes of $[Cu(pds)_2]^-$ anion.

ν n°	cm^{-1}	$I_{ir.}$	I_{Ra}	Symm.	Mode Assignment
7	108	0	48	Ag	δ(SeMSe)
11	194	0	35	Ag	v(4MSe) sy
12	227	0	8	B2g	butterfly wag
16	284	8	0	B3u	v(2MSe) asy
19	371	0	11	Ag	ring vibrations
21	378	19	0	B2u	ring vibrations
23	458	16	0	B1u	rings(6) wag
31	787	0	48	B1g	δ(CCN) +v(C-Se)
32	842	0	6	B2g	H wag
33	842	41	0	B1u	H wag
36	1058	31	0	B2u	δ(CCN) +v(C-Se)
38	1068	96	0	B3u	v(CC+CN)+ δ(HCC)... + v(C-Se)
39	1069	0	216	Ag	v(CC+CN)+ δ(HCC).. + v(C-Se)
40	1164	611	0	B3u	v(CC+CN)+ δ(HCC).. + v(C-Se)
41	1169	0	72	Ag	v(CC+CN)+ δ(HCC).. + v(C-Se)
44	1237	72	0	B3u	v(CC+CN)+ δ(HCC) + v(C-Se)
45	1240	0	140	Ag	v(CC+CN)+ δ(HCC) + v(C-Se)
46	1337	313	0	B3u	v(CC+CN)+ δ(HCC)
48	1445	0	43	B1g	v(CN)+ δ(HCC)
49	1447	19	0	B2u	v(CN)+ δ(HCC)
50	1509	0	322	B1g	v(CN)+ δ(HCC)
51	1510	19	0	B2u	v(CN)+ δ(HCC)
53	1561	0	249	Ag	v(CC+CN)+ δ(HCC)
54	3137	0	282	B1g	v2(CH)sym
56	3158	266	0	B3u	v2(CH)asym
57	3158	0	1516	Ag	v4(CH)sym

Table S4. Calculated frequencies of the most significant vibrational modes of $[Au(pds)_2]^-$ anion.

ν n°	cm^{-1}	$I_{ir.}$	I_{Ra}	Symm.	Mode Assignment
8	110	0	45	Ag	δ(SeMSe)
11	218	0	**27**	Ag	v(4MSe) sy
12	219	7	0	B2u	v(MSe) asy
13	228	0	8	B2g	butterfly wag
15	242	15	0	B3u	v(2MS) asy
19	368	0	15	Ag	ring vibrations
21	385	25	0	B2u	δ(SeCC)
22	475	0	2	B2g	rings(6) wag
23	476	14	0	B1u	rings(6) wag
26	625	4	0	B3u	δ(CNC)
27	626	0	4	Ag	δ(CNC)
29	790	0	65	B1g	δ(CCN) + v(C-Se)
33	870	69	0	B1u	H wag
38	1069	89	0	B3u	v(CC+CN) + δ(HCC)
39	1070	0	224	Ag	v(CC+CN) + δ(HCC) + v(C-Se)
40	1191	596	0	B3u	v(CC+CN) + δ(HCC) + v(C-Se)
41	1196	0	73	Ag	v(CC+CN) + δ(HCC) + v(C-Se)
44	1268	10	0	B3u	v(CC+CN)+ δ(HCC)
45	1269	0	3	Ag	v(CC+CN)+ δ(HCC)
46	1358	400	0	B3u	v(CC+CN)+ δ(HCC)
47	1361	0	14	Ag	v(CC+CN)+ δ(HCC)
48	1440	0	20	B1g	v(CC+CN)+ δ(HCC)
49	1441	42	0	B2u	v(CC+CN)+ δ(HCC)
50	1534	27	0	B2u	v(CN)+ δ(HCC)
51	1535	0	336	B1g	v(CN)+ δ(HCC)
52	1556	4	0	B3u	v(CC+CC)+ δ(HCC)
53	1557	0	135	Ag	v(CC+CN)+ δ(HCC)
55	3235	0	185	B1g	v2(CH)sym
56	3262	213	0	B3u	v2(CH)asym
57	3262	0	1036	Ag	v4(CH)sym

Table S5. IR[a] and Raman[b] peaks (cm^{-1}) of $(Bu_4N)[Cu(pdt)_2]$.

IR		RAMAN		Symmetry	Assignments
$\bar{\nu}_{obs}$	$\bar{\nu}_{calc}$ (Intensity)	$\bar{\nu}_{obs}$	$\bar{\nu}_{calc}$ (Intensity)		
		1535m	1522 (337)	B1g	ν(CN)+ δ(HCC)
1330s	1352 (478)			B3u	ν(CC+CN)+ δ(HCC)
		1332ms			
		not obs.	1274(151)	Ag	ν(CC+CN)+ δ(HCC)
	1188(752)	1199ms	1195(148)	Ag	ν(CC+CN+CS) + δ(HCC)
1191mw				B3u	ν(CC+CN+CS) + δ(HCC)
1143s					
1061w	1076(71)			B3u	ν(CC+CN+CS) + δ(HCC)
		1040w	1077(212)	Ag	ν(CC+CN+CS) + δ(HCC)
831w	839 (49)			B1u	Hwag
		not obs.	811(55)	B1g	δ(CCN)+ ν(CS)
480mw	461(22)	489w		B1u	Ring wag
442mw					
381mw	361(36)			B3u	ν_{as}(2CuS)
		344s	333(35)	Ag	ν_s(4CuS)
		223 w	252(9)	B2g	Butterfly wag
		122s	148(72)	Ag	δ(SCuS)

[a] Spectra recorded on KBr pellets. [b] Spectra recorded on solid samples mixed with KBr.

Table S6. IR[a] and Raman[b] peaks (cm^{-1}) of $(Bu_4N)[Cu(pds)_2]$.

IR		RAMAN		Symmetry	Assignments
$\bar{\nu}_{obs}$	$\bar{\nu}_{calc}$ (Intensity)	$\bar{\nu}_{obs}$	$\bar{\nu}_{calc}$ (Intensity)		
		1470w	1445 (43)	B1g	ν(CN)+ δ(HCC)
		1412w			
1318s	1337 (313)			B3u	ν(CC+CN)+ δ(HCC)
		1320w			
		not obs.	1240 (140)	Ag	ν(CC+CN+CSe) + δ(HCC)
		1179m	1169 (72)	Ag	ν(CC+CN+CSe) + δ(HCC)
1177m	1164 (611)			B3u	ν(CC+CN+CSe) + δ(HCC)
		1155m			
1133s					
1049,	1068 (96)			B3u	ν(CC+CN+CSe) + δ(HCC)
1041w	1058 (31)			B2u	ν(CSe) + δ(CCN)
		1050m	1069 (216)	Ag	ν(CC+CN+CSe) + δ(HCC)
841w	842 (41)			B1u	Hwag
		not obs.	749 (48)	B1g	δ(CCN)+ ν(CSe)
		489w			
437mw	458 (16)			B1u	Ring wag
378mw	378 (19)			B3u	ν_{as}(2CuSe)
		198s	227 (48)	B2g	Butterfly wag
		162m	194 (35)	Ag	ν_s(4CuSe)
		117vs	108 (48)	Ag	δ(SeCuSe)

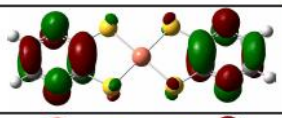
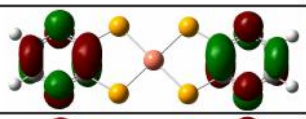
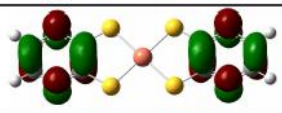
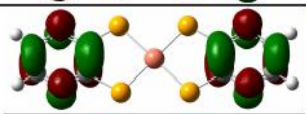
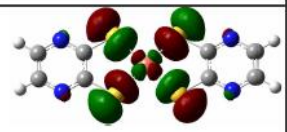
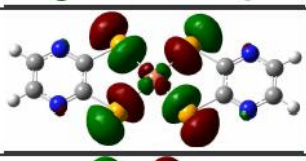
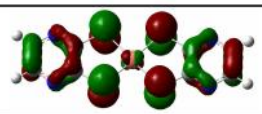
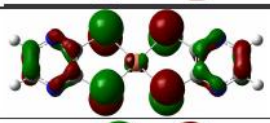
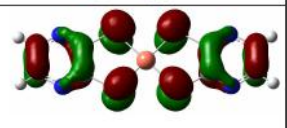
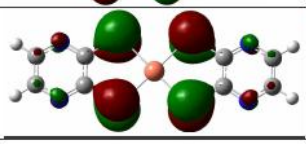
[a] Spectra recorded on KBr pellets. [b] Spectra recorded on solid samples mixed with KBr.

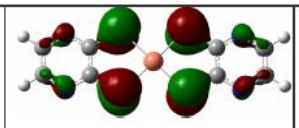
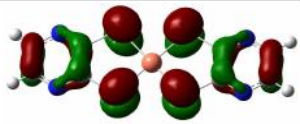
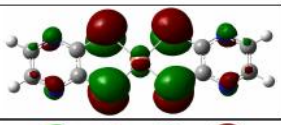
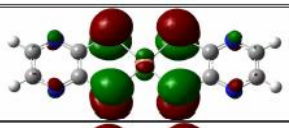
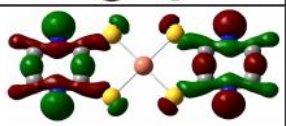
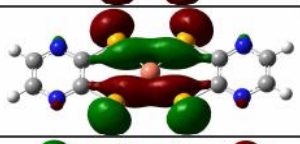
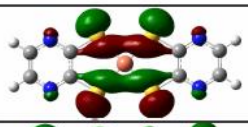
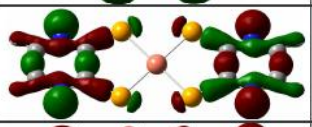
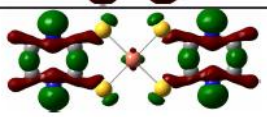
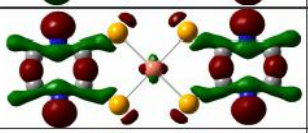
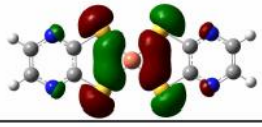
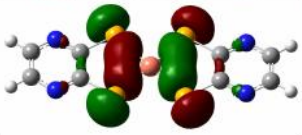
Table S7. IR[a] and Raman[b] peaks (cm^{-1}) of $(Bu_4N)[Au(pds)_2]$

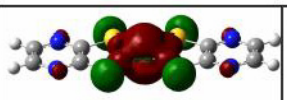
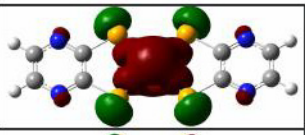
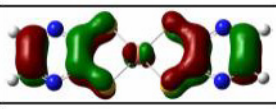
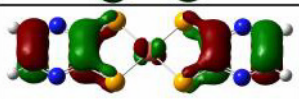
IR		RAMAN		Symmetry	Assignments
$\bar{\nu}_{obs}$	$\bar{\nu}_{calc}$ (Intensity)	$\bar{\nu}_{obs}$	$\bar{\nu}_{calc}$ (Intensity)		
		1527w	1535 (336)	B1g	ν(CN)+ δ(HCC)
		1477m	1440 (20)	B1g	ν(CC+CN)+ δ(HCC)
1319s	1358 (400)			B3u	ν(CC+CN)+ δ(HCC)
		1172mw	1196 (73)	Ag	ν(CC+CN+CSe) + δ(HCC)
		1134mw			
1171m	1191 (596)			B3u	ν(CC+CN+CSe) + δ(HCC)
1131s					
1042w	1069 (89)			B3u	ν(CC+CN) + δ(HCC)
		1050m	1070 (224)	Ag	ν(CC+CN+CSe) + δ(HCC)
879w	870 (69)			B1u	Hwag
843w					
		772w	790 (65)	B1g	δ(CCN)+ ν(CSe)
438mw	476 (14)			B1u	Ring wag
382mw	385 (25)			B2u	δ(SeCC)
350s					
not obs.	242 (15)			B3u	ν_{as}(2AuSe)
		258m			
		225ms	228 (8)	B2g	Butterfly wag
		179m	218 (27)	Ag	ν_s(4AuSe)
		116vs	110 (45)	Ag	δ(SeAuSe)

[a] Spectra recorded on KBr pellets. [b] Spectra recorded on a single crystal.

Table S8. Drawing, relative energy and symmetries of the most significant orbitals of $[Cu(pdt/s)]^-$ obtained by DFT calculations.

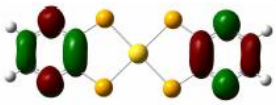
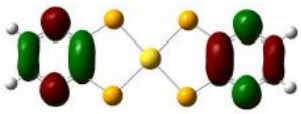
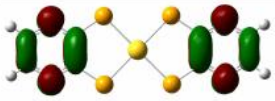
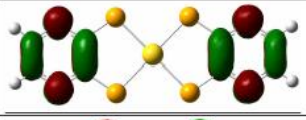
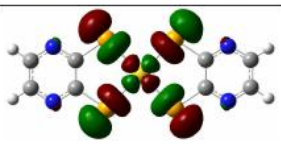
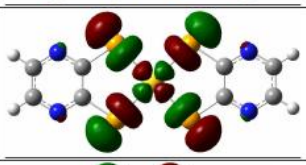
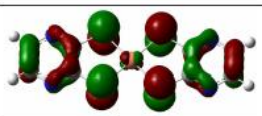
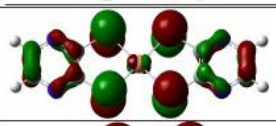
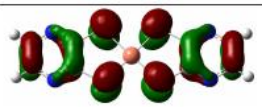
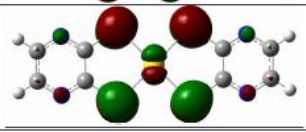
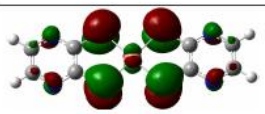
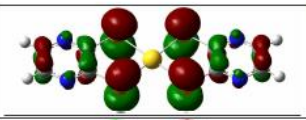
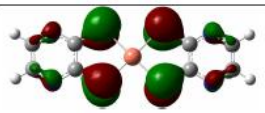
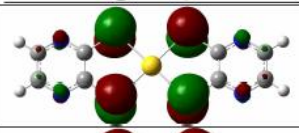
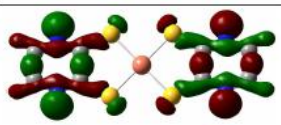
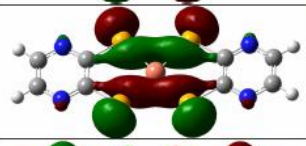
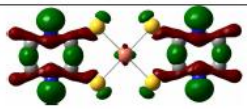
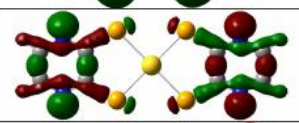
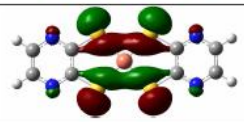
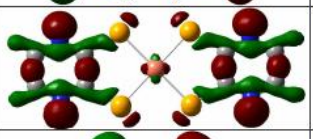
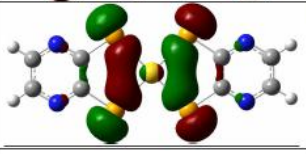
	$[Cu(pdt)_2]^{-1}$	E(eV)		$[Cu(pds)_2]^{-1}$			E(eV)
MO#n		**	Symm		MO#n	Symm	**
LUMO +2 #90		.060	B2g		LUMO+2 #126	B1u	.049
LUMO +1 #89		.054	B1u		LUMO+1 #125	B1u	.049
LUMO #88		-.008	B1g		LUMO #124	B1g	-.005
HOMO #87		-.101	B2g		HOMO #123	B2g	-0.099
HOMO-1 #86		-.133	B1u		HOMO-1 #122	Au	-.127

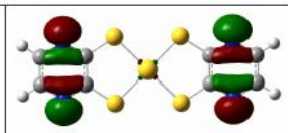
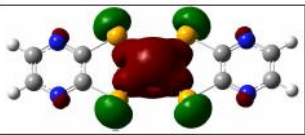
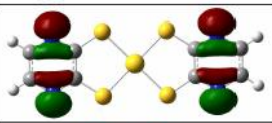
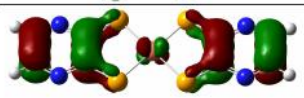
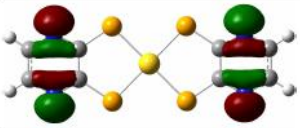
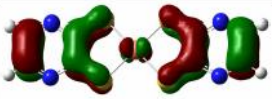
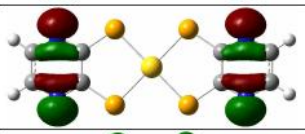
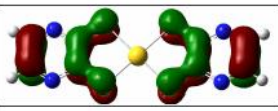
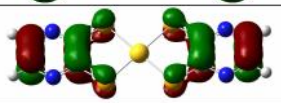
HOMO-2 #85		-.143	Au		HOMO-2 #121	B1u	-.132
HOMO-3 #84		-.149	B3g		HOMO-3 #120	B3g	-.136
HOMO-4 #83		-.153	B3u		HOMO-4 #119	B2u	-.143
HOMO-5 #82		-.156	B2u		HOMO-5 #118	B3u	-.152
HOMO-6 #81		-.157	Ag		HOMO-6 #117	Ag	-.158
HOMO-7 #80		-.188	B3u		HOMO-7 #116	B3u	-.174

HOMO-8 #79		-.218	Ag		HOMO-8 #115	Ag	-.210
HOMO-9 #78		-.218	B2g		HOMO-9 #114	B2g	-.212

** E da OPT PBE1PBE/6-311++G(2df,2p)

Table S9. Drawing, relative energy and symmetries of the most significant orbitals of $[Au(pdt/s)]^{-}$ obtained by DFT calculations.

	$[Au(pdt)_2]^{-1}$	E(eV)		$[Au(pds)_2]^{-1}$			E(eV)
MO#n		**	Symm		MO#n	Symm	**
LUMO +2 #85		.052	B2g		LUMO+2 #65	B1u	.048
LUMO +1 #84		.049	B1u		LUMO+1 #64	B1u	.045
LUMO #83		.000	B1g		LUMO #63	B1g	.004
HOMO #82		-.108	B2g		HOMO #62	B2g	-0.100
HOMO-1 #81		-.138	B1u		HOMO-1 #61	B3g	-.131
HOMO-2 #80		-.146	B3g		HOMO-2 #60	B1u	-.132
HOMO-3 #79		-.153	Au		HOMO-3 #59	Au	-.134
HOMO-4 #78		-.155	B3u		HOMO-4 #58	B2u	-.151
HOMO-5 #77		-.156	Ag		HOMO-5 #57	B3u	-.152
HOMO-6 #76		-.163	B2u		HOMO-6 #56	Ag	-.155
HOMO-7 #75		-.190	B3u		HOMO-7 #55	B3u	-.174

HOMO-8 #74		-.218	B1g		HOMO-8 #54	Ag	-.217
HOMO-9 #73		-.220	B2u		HOMO-9 #53	B2g	-.218
HOMO-10 #72		-.221	Ag		HOMO-10 #52	B1g	-.220
HOMO-11 #71		-.224	B2g		HOMO-11 #51	B2u	-.221
HOMO-12 #70		-.237	B1u		HOMO-121 #50	B1u	-.227

** E da OPT PBE1PBE/SDD

Table S10. Drawing, relative energy and symmetries of the most significant orbitals of $[Ni(pdt/s)]^{2-}$ obtained by DFT calculations.

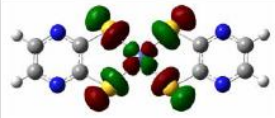
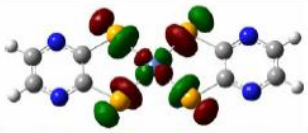
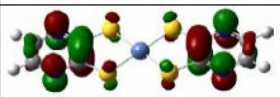
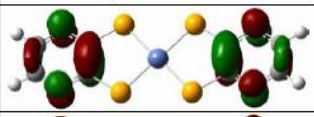
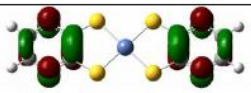
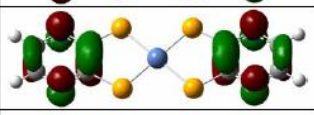
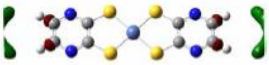
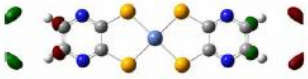
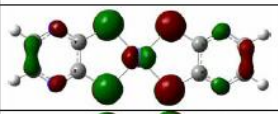
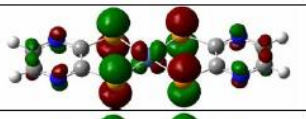
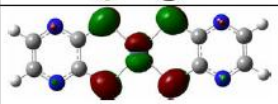
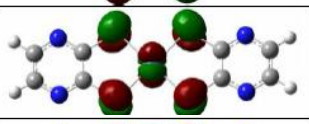
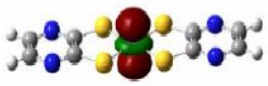
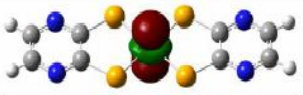
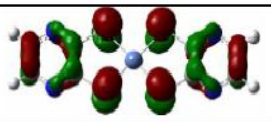
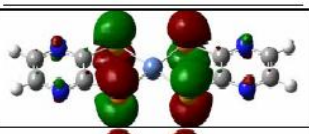
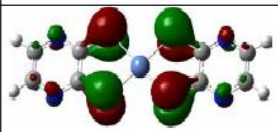
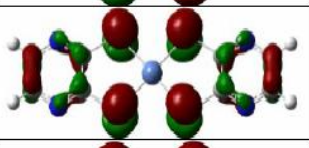
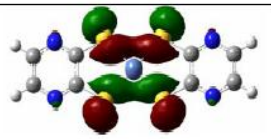
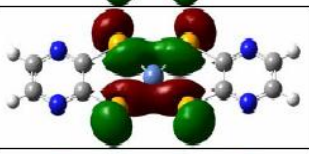
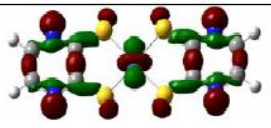
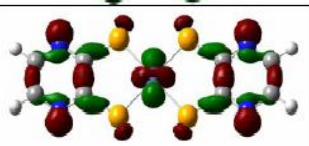
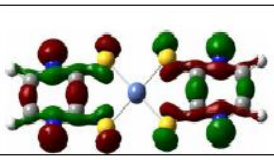
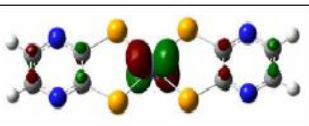
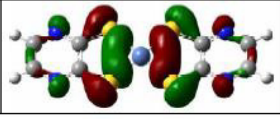
	$[Ni(pdt)_2]^{--}$	E(eV)		$[Ni(pds)_2]^{---}$			E(eV)
MO#n		**	Symm		MO#n	Symm	**
LUMO +9 #97		0.21162	Au		LUMO+n #131	Au	0.20078
LUMO +6 #94		0.18827	B2g		LUMO+n #130	B2g	0.17659
LUMO +4 #92		0.17982	B1u		LUMO+2 #126	B1u	0.17088
LUMO #88		0.15173	Ag		LUMO #124	B3u	0.14854
HOMO #87		0.04995	B2g		HOMO #123	B2g	0.04602
HOMO-1 #86		0.01980	B1g		HOMO-1 #122	B1g	0.02263
HOMO-2 #85		0.01001	Ag		HOMO-2 #121	Ag	0.00994
HOMO-3 #84		0.00701	B1u		HOMO-3 #120	Au	0.00777
HOMO-4 #83		-0.00309	Au		HOMO-4 #119	B1u	0.00187
HOMO-5 #82		-0.00608	B2u		HOMO-5 #118	B2u	0.00064
HOMO-6 #81		-0.01990	Ag		HOMO-6 #117	Ag	-0.02225
HOMO-7 #80		-0.02263	B3u		HOMO-7 #116	B2g	-0.02776
HOMO-9 #78		-0.04120	B3u				

Table S11. Cartesian coordinates for $[M(pdt/s)_2]^z$ (z = 0, 1–, 2–; M = Ni, Cu, Au).

$[Ni(pdt)_2]^0$ E(au)=-3626.18733 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.705700	5.198629
2	6	0	0.000000	0.710830	2.943081
3	6	0	0.000000	-0.710830	2.943081
4	6	0	0.000000	-0.705700	5.198629
5	1	0	0.000000	1.253931	6.135336
6	1	0	0.000000	-1.253931	6.135336
7	16	0	0.000000	-1.554663	1.464001
8	16	0	0.000000	1.554663	1.464001
9	1	0	0.000000	-1.253931	-6.135336
10	6	0	0.000000	-0.705700	-5.198629
11	6	0	0.000000	0.705700	-5.198629
12	1	0	0.000000	1.253931	-6.135336
13	6	0	0.000000	-0.710830	-2.943081
14	6	0	0.000000	0.710830	-2.943081
15	16	0	0.000000	-1.554663	-1.464001
16	16	0	0.000000	1.554663	-1.464001
17	7	0	0.000000	-1.405771	4.091340
18	7	0	0.000000	1.405771	4.091340
19	7	0	0.000000	-1.405771	-4.091340
20	7	0	0.000000	1.405771	-4.091340
21	28	0	0.000000	0.000000	0.000000

$[Ni(pdt)_2]^{1-}$ E(au)=-3626.32957 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.692631	5.270232
2	6	0	0.000000	0.710499	3.007123
3	6	0	0.000000	-0.710499	3.007123
4	6	0	0.000000	-0.692631	5.270232
5	1	0	0.000000	1.251144	6.201627
6	1	0	0.000000	-1.251144	6.201627
7	16	0	0.000000	-1.558152	1.501195
8	16	0	0.000000	1.558152	1.501195
9	1	0	0.000000	-1.251144	-6.201627
10	6	0	0.000000	-0.692631	-5.270232
11	6	0	0.000000	0.692631	-5.270232
12	1	0	0.000000	1.251144	-6.201627
13	6	0	0.000000	-0.710499	-3.007123
14	6	0	0.000000	0.710499	-3.007123
15	16	0	0.000000	-1.558152	-1.501195
16	16	0	0.000000	1.558152	-1.501195
17	7	0	0.000000	-1.396977	4.143306
18	7	0	0.000000	1.396977	4.143306
19	7	0	0.000000	-1.396977	-4.143306
20	7	0	0.000000	1.396977	-4.143306
21	28	0	0.000000	0.000000	0.000000

$[Ni(pdt)_2]^{2-}$ E(au)=-3626.31632 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.687605	5.326481
2	6	0	0.000000	0.720710	3.049469
3	6	0	0.000000	-0.720710	3.049469
4	6	0	0.000000	-0.687605	5.326481
5	1	0	0.000000	1.248088	6.259759
6	1	0	0.000000	-1.248088	6.259759
7	16	0	0.000000	-1.563955	1.543259
8	16	0	0.000000	1.563955	1.543259
9	1	0	0.000000	-1.248088	-6.259759
10	6	0	0.000000	-0.687605	-5.326481
11	6	0	0.000000	0.687605	-5.326481
12	1	0	0.000000	1.248088	-6.259759
13	6	0	0.000000	-0.720710	-3.049469
14	6	0	0.000000	0.720710	-3.049469
15	16	0	0.000000	-1.563955	-1.543259
16	16	0	0.000000	1.563955	-1.543259
17	7	0	0.000000	-1.398257	4.191540
18	7	0	0.000000	1.398257	4.191540
19	7	0	0.000000	-1.398257	-4.191540
20	7	0	0.000000	1.398257	-4.191540
21	28	0	0.000000	0.000000	0.000000

$[Ni(pds)_2]^0$ E(au)=-11638.85065 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.702904	5.389202
2	6	0	0.000000	0.706890	3.131093
3	6	0	0.000000	-0.706890	3.131093
4	6	0	0.000000	-0.702904	5.389202
5	1	0	0.000000	1.255150	6.323290
6	1	0	0.000000	-1.255150	6.323290
7	1	0	0.000000	-1.255150	-6.323290
8	6	0	0.000000	-0.702904	-5.389202
9	6	0	0.000000	0.702904	-5.389202
10	1	0	0.000000	1.255150	-6.323290
11	6	0	0.000000	-0.706890	-3.131093
12	6	0	0.000000	0.706890	-3.131093
13	7	0	0.000000	-1.399123	4.276077
14	7	0	0.000000	1.399123	4.276077
15	7	0	0.000000	-1.399123	-4.276077
16	7	0	0.000000	1.399123	-4.276077
17	34	0	0.000000	-1.651797	1.533969
18	34	0	0.000000	1.651797	1.533969
19	34	0	0.000000	-1.651797	-1.533969
20	34	0	0.000000	1.651797	-1.533969
21	28	0	0.000000	0.000000	0.000000

$[Ni(pds)_2]^{1-}$ E(au)=-11638.99390 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.691156	5.476905
2	6	0	0.000000	0.707730	3.212272
3	6	0	0.000000	-0.707730	3.212272
4	6	0	0.000000	-0.691156	5.476905
5	1	0	0.000000	1.253307	6.405798
6	1	0	0.000000	-1.253307	6.405798
7	1	0	0.000000	-1.253307	-6.405798
8	6	0	0.000000	-0.691156	-5.476905
9	6	0	0.000000	0.691156	-5.476905
10	1	0	0.000000	1.253307	-6.405798
11	6	0	0.000000	-0.707730	-3.212272
12	6	0	0.000000	0.707730	-3.212272
13	7	0	0.000000	-1.392166	4.345534
14	7	0	0.000000	1.392166	4.345534
15	7	0	0.000000	-1.392166	-4.345534
16	7	0	0.000000	1.392166	-4.345534
17	34	0	0.000000	-1.655590	1.588723
18	34	0	0.000000	1.655590	1.588723
19	34	0	0.000000	-1.655590	-1.588723
20	34	0	0.000000	1.655590	-1.588723
21	28	0	0.000000	0.000000	0.000000

$[Ni(pds)_2]^{2-}$ E(au)=-11638.97947 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.688018	5.525754
2	6	0	0.000000	0.717368	3.249015
3	6	0	0.000000	-0.717368	3.249015
4	6	0	0.000000	-0.688018	5.525754
5	1	0	0.000000	1.250156	6.457755
6	1	0	0.000000	-1.250156	6.457755
7	1	0	0.000000	-1.250156	-6.457755
8	6	0	0.000000	-0.688018	-5.525754
9	6	0	0.000000	0.688018	-5.525754
10	1	0	0.000000	1.250156	-6.457755
11	6	0	0.000000	-0.717368	-3.249015
12	6	0	0.000000	0.717368	-3.249015
13	7	0	0.000000	-1.394293	4.389693
14	7	0	0.000000	1.394293	4.389693
15	7	0	0.000000	-1.394293	-4.389693
16	7	0	0.000000	1.394293	-4.389693
17	34	0	0.000000	-1.654700	1.622950
18	34	0	0.000000	1.654700	1.622950
19	34	0	0.000000	-1.654700	-1.622950
20	34	0	0.000000	1.654700	-1.622950
21	28	0	0.000000	0.000000	0.000000

$[Cu(pdt)_2]^0$ E(au)=-3758.35136 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.699514	5.232314
2	6	0	0.000000	0.707578	2.975482
3	6	0	0.000000	-0.707578	2.975482
4	6	0	0.000000	-0.699514	5.232314
5	1	0	0.000000	1.255615	6.163500
6	1	0	0.000000	-1.255615	6.163500
7	16	0	0.000000	-1.586793	1.494446
8	16	0	0.000000	1.586793	1.494446
9	1	0	0.000000	-1.255615	-6.163500
10	6	0	0.000000	-0.699514	-5.232314
11	6	0	0.000000	0.699514	-5.232314
12	1	0	0.000000	1.255615	-6.163500
13	6	0	0.000000	-0.707578	-2.975482
14	6	0	0.000000	0.707578	-2.975482
15	16	0	0.000000	-1.586793	-1.494446
16	16	0	0.000000	1.586793	-1.494446
17	29	0	0.000000	0.000000	0.000000
18	7	0	0.000000	-1.397466	4.112357
19	7	0	0.000000	1.397466	4.112357
20	7	0	0.000000	-1.397466	-4.112357
21	7	0	0.000000	1.397466	-4.112357

$[Cu(pdt)_2]^{1-}$ E(au)=-3758.49724 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.689014	5.297961
2	6	0	0.000000	0.709351	3.033419
3	6	0	0.000000	-0.709351	3.033419
4	6	0	0.000000	-0.689014	5.297961
5	1	0	0.000000	1.252063	6.226011
6	1	0	0.000000	-1.252063	6.226011
7	16	0	0.000000	-1.578066	1.527303
8	16	0	0.000000	1.578066	1.527303
9	1	0	0.000000	-1.252063	-6.226011
10	6	0	0.000000	-0.689014	-5.297961
11	6	0	0.000000	0.689014	-5.297961
12	1	0	0.000000	1.252063	-6.226011
13	6	0	0.000000	-0.709351	-3.033419
14	6	0	0.000000	0.709351	-3.033419
15	16	0	0.000000	-1.578066	-1.527303
16	16	0	0.000000	1.578066	-1.527303
17	29	0	0.000000	0.000000	0.000000
18	7	0	0.000000	-1.392840	4.162637
19	7	0	0.000000	1.392840	4.162637
20	7	0	0.000000	-1.392840	-4.162637
21	7	0	0.000000	1.392840	-4.162637

$[Cu(pdt)_2]^{2-}$ E(au)=-3758.47762 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.687086	5.414758
2	6	0	0.000000	0.723981	3.129573
3	6	0	0.000000	-0.723981	3.129573
4	6	0	0.000000	-0.687086	5.414758
5	1	0	0.000000	1.250066	6.346813
6	1	0	0.000000	-1.250066	6.346813
7	16	0	0.000000	-1.615252	1.648666
8	16	0	0.000000	1.615252	1.648666
9	1	0	0.000000	-1.250066	-6.346813
10	6	0	0.000000	-0.687086	-5.414758
11	6	0	0.000000	0.687086	-5.414758
12	1	0	0.000000	1.250066	-6.346813
13	6	0	0.000000	-0.723981	-3.129573
14	6	0	0.000000	0.723981	-3.129573
15	16	0	0.000000	-1.615252	-1.648666
16	16	0	0.000000	1.615252	-1.648666
17	29	0	0.000000	0.000000	0.000000
18	7	0	0.000000	-1.392269	4.278905
19	7	0	0.000000	1.392269	4.278905
20	7	0	0.000000	-1.392269	-4.278905
21	7	0	0.000000	1.392269	-4.278905

$[Cu(pds)_2]^{0}$ E(au)=-11771.02915 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.697895	5.425310
2	6	0	0.000000	0.705554	3.165188
3	6	0	0.000000	-0.705554	3.165188
4	6	0	0.000000	-0.697895	5.425310
5	1	0	0.000000	1.257832	6.354022
6	1	0	0.000000	-1.257832	6.354022
7	1	0	0.000000	-1.257832	-6.354022
8	6	0	0.000000	-0.697895	-5.425310
9	6	0	0.000000	0.697895	-5.425310
10	1	0	0.000000	1.257832	-6.354022
11	6	0	0.000000	-0.705554	-3.165188
12	6	0	0.000000	0.705554	-3.165188
13	7	0	0.000000	-1.391898	4.300750
14	7	0	0.000000	1.391898	4.300750
15	7	0	0.000000	-1.391898	-4.300750
16	7	0	0.000000	1.391898	-4.300750
17	34	0	0.000000	-1.685779	1.571458
18	34	0	0.000000	1.685779	1.571458
19	34	0	0.000000	-1.685779	-1.571458
20	34	0	0.000000	1.685779	-1.571458
21	29	0	0.000000	0.000000	0.000000

$[Cu(pds)_2]^{1-}$ E(au)=-11771.17091 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.689069	5.497811
2	6	0	0.000000	0.707432	3.231258
3	6	0	0.000000	-0.707432	3.231258
4	6	0	0.000000	-0.689069	5.497811
5	1	0	0.000000	1.254107	6.424742
6	1	0	0.000000	-1.254107	6.424742
7	1	0	0.000000	-1.254107	-6.424742
8	6	0	0.000000	-0.689069	-5.497811
9	6	0	0.000000	0.689069	-5.497811
10	1	0	0.000000	1.254107	-6.424742
11	6	0	0.000000	-0.707432	-3.231258
12	6	0	0.000000	0.707432	-3.231258
13	29	0	0.000000	0.000000	0.000000
14	7	0	0.000000	-1.389229	4.360904
15	7	0	0.000000	1.389229	4.360904
16	7	0	0.000000	-1.389229	-4.360904
17	7	0	0.000000	1.389229	-4.360904
18	34	0	0.000000	-1.670894	1.612044
19	34	0	0.000000	1.670894	1.612044
20	34	0	0.000000	-1.670894	-1.612044
21	34	0	0.000000	1.670894	-1.612044

$[Cu(pds)]^{2-}$ E(au)=-11771.14629 PBE1PBE/6-311++G(2df,2p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.687726	5.613478
2	6	0	0.000000	0.719652	3.330099
3	6	0	0.000000	-0.719652	3.330099
4	6	0	0.000000	-0.687726	5.613478
5	1	0	0.000000	1.252606	6.544017
6	1	0	0.000000	-1.252606	6.544017
7	1	0	0.000000	-1.252606	-6.544017
8	6	0	0.000000	-0.687726	-5.613478
9	6	0	0.000000	0.687726	-5.613478
10	1	0	0.000000	1.252606	-6.544017
11	6	0	0.000000	-0.719652	-3.330099
12	6	0	0.000000	0.719652	-3.330099
13	7	0	0.000000	-1.388786	4.476824
14	7	0	0.000000	1.388786	4.476824
15	7	0	0.000000	-1.388786	-4.476824
16	7	0	0.000000	1.388786	-4.476824
17	34	0	0.000000	-1.708805	1.731166
18	34	0	0.000000	1.708805	1.731166
19	34	0	0.000000	-1.708805	-1.731166
20	34	0	0.000000	1.708805	-1.731166
21	29	0	0.000000	0.000000	0.000000

$[Au(pdt)_2]^0$ E(au)=-2253.35434 PBE1PBE/SDD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.706464	5.469083
2	6	0	0.000000	0.711813	3.159990
3	6	0	0.000000	-0.711813	3.159990
4	6	0	0.000000	-0.706464	5.469083
5	1	0	0.000000	1.275159	6.391854
6	1	0	0.000000	-1.275159	6.391854
7	16	0	0.000000	-1.693837	1.671869
8	16	0	0.000000	1.693837	1.671869
9	1	0	0.000000	-1.275159	-6.391854
10	6	0	0.000000	-0.706464	-5.469083
11	6	0	0.000000	0.706464	-5.469083
12	1	0	0.000000	1.275159	-6.391854
13	6	0	0.000000	-0.711813	-3.159990
14	6	0	0.000000	0.711813	-3.159990
15	16	0	0.000000	-1.693837	-1.671869
16	16	0	0.000000	1.693837	-1.671869
17	79	0	0.000000	0.000000	0.000000
18	7	0	0.000000	1.402637	4.321071
19	7	0	0.000000	-1.402637	4.321071
20	7	0	0.000000	1.402637	-4.321071
21	7	0	0.000000	-1.402637	-4.321071

$[Au(pdt)_2]^{1-}$ E(au)=-2253.51142 PBE1PBE/SDD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-0.698434	5.519443
2	6	0	0.000000	-0.714568	3.203118
3	6	0	0.000000	0.714568	3.203118
4	6	0	0.000000	0.698434	5.519443
5	1	0	0.000000	-1.273658	6.439519
6	1	0	0.000000	1.273658	6.439519
7	16	0	0.000000	1.691266	1.697681
8	16	0	0.000000	-1.691266	1.697681
9	1	0	0.000000	1.273658	-6.439519
10	6	0	0.000000	0.698434	-5.519443
11	6	0	0.000000	-0.698434	-5.519443
12	1	0	0.000000	-1.273658	-6.439519
13	6	0	0.000000	0.714568	-3.203118
14	6	0	0.000000	-0.714568	-3.203118
15	16	0	0.000000	1.691266	-1.697681
16	16	0	0.000000	-1.691266	-1.697681
17	79	0	0.000000	0.000000	0.000000
18	7	0	0.000000	-1.400081	4.360353
19	7	0	0.000000	1.400081	4.360353
20	7	0	0.000000	-1.400081	-4.360353
21	7	0	0.000000	1.400081	-4.360353

$[Au(pdt)_2]^{2-}$ E(au) = -2253.47544 PBE1PBE/SDD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.696536	5.682174
2	6	0	0.000000	0.727581	3.346822
3	6	0	0.000000	-0.727581	3.346822
4	6	0	0.000000	-0.696536	5.682174
5	1	0	0.000000	1.274073	6.604407
6	1	0	0.000000	-1.274073	6.604407
7	16	0	0.000000	-1.710350	1.861538
8	16	0	0.000000	1.710350	1.861538
9	1	0	0.000000	-1.274073	-6.604407
10	6	0	0.000000	-0.696536	-5.682174
11	6	0	0.000000	0.696536	-5.682174
12	1	0	0.000000	1.274073	-6.604407
13	6	0	0.000000	-0.727581	-3.346822
14	6	0	0.000000	0.727581	-3.346822
15	16	0	0.000000	-1.710350	-1.861538
16	16	0	0.000000	1.710350	-1.861538
17	79	0	0.000000	0.000000	0.000000
18	7	0	0.000000	1.401678	4.521957
19	7	0	0.000000	-1.401678	4.521957
20	7	0	0.000000	1.401678	-4.521957
21	7	0	0.000000	-1.401678	-4.521957

$[Au(pds)_2]^{0}$ E(au)=-698.71854 PBE1PBE/SDD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.705645	5.618675
2	6	0	0.000000	0.711598	3.304244
3	6	0	0.000000	-0.711598	3.304244
4	6	0	0.000000	-0.705645	5.618675
5	1	0	0.000000	1.275279	6.540814
6	1	0	0.000000	-1.275279	6.540814
7	1	0	0.000000	-1.275279	-6.540814
8	6	0	0.000000	-0.705645	-5.618675
9	6	0	0.000000	0.705645	-5.618675
10	1	0	0.000000	1.275279	-6.540814
11	6	0	0.000000	-0.711598	-3.304244
12	6	0	0.000000	0.711598	-3.304244
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.401289	4.468586
15	7	0	0.000000	-1.401289	4.468586
16	7	0	0.000000	1.401289	-4.468586
17	7	0	0.000000	-1.401289	-4.468586
18	34	0	0.000000	1.784012	1.728067
19	34	0	0.000000	-1.784012	1.728067
20	34	0	0.000000	-1.784012	-1.728067
21	34	0	0.000000	1.784012	-1.728067

$[Au(pds)_2]^{1-}$ E(au)=-698.86542 PBE1PBE/SDD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.699004	5.677492
2	6	0	0.000000	0.715143	3.357456
3	6	0	0.000000	-0.715143	3.357456
4	6	0	0.000000	-0.699004	5.677492
5	1	0	0.000000	1.273480	6.597933
6	1	0	0.000000	-1.273480	6.597933
7	1	0	0.000000	-1.273480	-6.597933
8	6	0	0.000000	-0.699004	-5.677492
9	6	0	0.000000	0.699004	-5.677492
10	1	0	0.000000	1.273480	-6.597933
11	6	0	0.000000	-0.715143	-3.357456
12	6	0	0.000000	0.715143	-3.357456
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.400289	4.518085
15	7	0	0.000000	-1.400289	4.518085
16	7	0	0.000000	1.400289	-4.518085
17	7	0	0.000000	-1.400289	-4.518085
18	34	0	0.000000	1.777144	1.759873
19	34	0	0.000000	-1.777144	1.759873
20	34	0	0.000000	-1.777144	-1.759873
21	34	0	0.000000	1.777144	-1.759873

$[Au(pds)_2]^{2-}$ E(au)=-698.82525 PBE1PBE/SDD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.697389	5.827155
2	6	0	0.000000	0.726412	3.490887
3	6	0	0.000000	-0.726412	3.490887
4	6	0	0.000000	-0.697389	5.827155
5	1	0	0.000000	1.273921	6.749455
6	1	0	0.000000	-1.273921	6.749455
7	1	0	0.000000	-1.273921	-6.749455
8	6	0	0.000000	-0.697389	-5.827155
9	6	0	0.000000	0.697389	-5.827155
10	1	0	0.000000	1.273921	-6.749455
11	6	0	0.000000	-0.726412	-3.490887
12	6	0	0.000000	0.726412	-3.490887
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.401332	4.667244
15	7	0	0.000000	-1.401332	4.667244
16	7	0	0.000000	1.401332	-4.667244
17	7	0	0.000000	-1.401332	-4.667244
18	34	0	0.000000	1.798219	1.904825
19	34	0	0.000000	-1.798219	1.904825
20	34	0	0.000000	-1.798219	-1.904825
21	34	0	0.000000	1.798219	-1.904825

[Au(pdt)$_2$]^0 E(au)=-2253.74970 PBE1PBE// 6-311++G(2df,2p)for **C N H S (Se)**, (aug-cc-pVTZ-PP) for Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.702302	5.346054
2	6	0	0.000000	0.710899	3.075981
3	6	0	0.000000	-0.710899	3.075981
4	6	0	0.000000	-0.702302	5.346054
5	1	0	0.000000	1.262690	6.277825
6	1	0	0.000000	-1.262690	6.277825
7	1	0	0.000000	-1.262690	-6.277825
8	6	0	0.000000	-0.702302	-5.346054
9	6	0	0.000000	0.702302	-5.346054
10	1	0	0.000000	1.262690	-6.277825
11	6	0	0.000000	-0.710899	-3.075981
12	6	0	0.000000	0.710899	-3.075981
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.401544	4.221744
15	7	0	0.000000	-1.401544	4.221744
16	7	0	0.000000	1.401544	-4.221744
17	7	0	0.000000	-1.401544	-4.221744
18	16	0	0.000000	1.641415	1.622330
19	16	0	0.000000	-1.641415	1.622330
20	16	0	0.000000	-1.641415	-1.622330
21	16	0	0.000000	1.641415	-1.622330

[Au(pdt)$_2$]$^{-1}$ E(au)=-2253.89147 PBE1PBE// 6-311++G(2df,2p)for **C N H S (Se)**, (aug-cc-pVTZ-PP) for Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.692957	5.400228
2	6	0	0.000000	0.713641	3.121386
3	6	0	0.000000	-0.713641	3.121386
4	6	0	0.000000	-0.692957	5.400228
5	1	0	0.000000	1.260618	6.328822
6	1	0	0.000000	-1.260618	6.328822
7	1	0	0.000000	-1.260618	-6.328822
8	6	0	0.000000	-0.692957	-5.400228
9	6	0	0.000000	0.692957	-5.400228
10	1	0	0.000000	1.260618	-6.328822
11	6	0	0.000000	-0.713641	-3.121386
12	6	0	0.000000	0.713641	-3.121386
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.396468	4.261851
15	7	0	0.000000	-1.396468	4.261851
16	7	0	0.000000	1.396468	-4.261851
17	7	0	0.000000	-1.396468	-4.261851
18	16	0	0.000000	1.642623	1.648212
19	16	0	0.000000	-1.642623	1.648212
20	16	0	0.000000	-1.642623	-1.648212
21	16	0	0.000000	1.642623	-1.648212

[Au(pdt)$_2$]$^{-2}$ E(au)=-2253.83627 PBE1PBE// 6-311++G(2df,2p)for **C N H S (Se)**, (aug-cc-pVTZ-PP) for Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.691249	5.551927
2	6	0	0.000000	0.727354	3.253942
3	6	0	0.000000	-0.727354	3.253942
4	6	0	0.000000	-0.691249	5.551927
5	1	0	0.000000	1.259792	6.483841
6	1	0	0.000000	-1.259792	6.483841
7	1	0	0.000000	-1.259792	-6.483841
8	6	0	0.000000	-0.691249	-5.551927
9	6	0	0.000000	0.691249	-5.551927
10	1	0	0.000000	1.259792	-6.483841
11	6	0	0.000000	-0.727354	-3.253942
12	6	0	0.000000	0.727354	-3.253942
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.396254	4.412786
15	7	0	0.000000	-1.396254	4.412786
16	7	0	0.000000	1.396254	-4.412786
17	7	0	0.000000	-1.396254	-4.412786
18	16	0	0.000000	1.667164	1.800459
19	16	0	0.000000	-1.667164	1.800459
20	16	0	0.000000	-1.667164	-1.800459
21	16	0	0.000000	1.667164	-1.800459

[Au(pds)$_2$]^{0} E(au)=-10266.55149 PBE1PBE// 6-311++G(2df,2p)for **C N H S (Se)**, (aug-cc-pVTZ-PP) for Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.697869	5.518981
2	6	0	0.000000	0.705564	3.254057
3	6	0	0.000000	-0.705564	3.254057
4	6	0	0.000000	-0.697869	5.518981
5	1	0	0.000000	1.259885	6.448261
6	1	0	0.000000	-1.259885	6.448261
7	1	0	0.000000	-1.259885	-6.448261
8	6	0	0.000000	-0.697869	-5.518981
9	6	0	0.000000	0.697869	-5.518981
10	1	0	0.000000	1.259885	-6.448261
11	6	0	0.000000	-0.705564	-3.254057
12	6	0	0.000000	0.705564	-3.254057
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.390520	4.394274
15	7	0	0.000000	-1.390520	4.394274
16	7	0	0.000000	1.390520	-4.394274
17	7	0	0.000000	-1.390520	-4.394274
18	34	0	0.000000	1.738988	1.690654
19	34	0	0.000000	-1.738988	1.690654
20	34	0	0.000000	-1.738988	-1.690654
21	34	0	0.000000	1.738988	-1.690654

[Au(pds)$_2$]$^{-1}$ E(au)=-10266.70796 PBE1PBE// 6-311++G(2df,2p)for **C N H S (Se)**, (aug-cc-pVTZ-PP) for Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.689338	5.579413
2	6	0	0.000000	0.708374	3.307779
3	6	0	0.000000	-0.708374	3.307779
4	6	0	0.000000	-0.689338	5.579413
5	1	0	0.000000	1.255596	6.505541
6	1	0	0.000000	-1.255596	6.505541
7	1	0	0.000000	-1.255596	-6.505541
8	6	0	0.000000	-0.689338	-5.579413
9	6	0	0.000000	0.689338	-5.579413
10	1	0	0.000000	1.255596	-6.505541
11	6	0	0.000000	-0.708374	-3.307779
12	6	0	0.000000	0.708374	-3.307779
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.385823	4.443082
15	7	0	0.000000	-1.385823	4.443082
16	7	0	0.000000	1.385823	-4.443082
17	7	0	0.000000	-1.385823	-4.443082
18	34	0	0.000000	1.733710	1.723866
19	34	0	0.000000	-1.733710	1.723866
20	34	0	0.000000	-1.733710	-1.723866
21	34	0	0.000000	1.733710	-1.723866

[Au(pds)$_2$]$^{-2}$ E(au)=-10266.51388 PBE1PBE// 6-311++G(2df,2p)for **C N H S (Se)**, (aug-cc-pVTZ-PP) for Au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.691598	5.736096
2	6	0	0.000000	0.723066	3.440318
3	6	0	0.000000	-0.723066	3.440318
4	6	0	0.000000	-0.691598	5.736096
5	1	0	0.000000	1.261387	6.666816
6	1	0	0.000000	-1.261387	6.666816
7	1	0	0.000000	-1.261387	-6.666816
8	6	0	0.000000	-0.691598	-5.736096
9	6	0	0.000000	0.691598	-5.736096
10	1	0	0.000000	1.261387	-6.666816
11	6	0	0.000000	-0.723066	-3.440318
12	6	0	0.000000	0.723066	-3.440318
13	79	0	0.000000	0.000000	0.000000
14	7	0	0.000000	1.393656	4.595953
15	7	0	0.000000	-1.393656	4.595953
16	7	0	0.000000	1.393656	-4.595953
17	7	0	0.000000	-1.393656	-4.595953
18	34	0	0.000000	1.762797	1.871148
19	34	0	0.000000	-1.762797	1.871148
20	34	0	0.000000	-1.762797	-1.871148
21	34	0	0.000000	1.762797	-1.871148