Electronic Supplementary Material (ESI) for ChemComm.

A radical mixed-ligand gold bis(dithiolene) complex

Romain Perochon, Frédéric Barrière, Olivier Jeannin, Lidia Piekara-Sady and Marc Fourmigué

Electronic Supplementary Information (ESI)

Synthesis of [Au(*D*-bordt)(OC_4)] (1)

To a solution of [Au(*D*-bordt)$_2$] (116 mg, 0.19 mmol) in dry THF (100 mL) is added a solution of [Au(OC4)$_2$] (189 mg, 0.19 mmol) in THF (100 mL). After refluxing for 3 days, the solvent is evaporated and the residue separated from the starting complexes by preparative thin-layer chromatography. Recrystallization by slow diffusion of MeOH on a concentrated CH_2Cl_2 solution afforded **1** as black crystals (102 mg). Yield 33%. M.p. 109 °C. Elem. Anal. Calcd. for $C_{32}H_{40}AuO_2S_4$: C, 49.16; H, 5.16. Found : C, 49.17; H, 4.86. UV–vis–NIR (CH_2Cl_2): λ_{max} = 1347 nm ($\varepsilon = 7\,130\ M^{-1}\ cm^{-1}$). $[\alpha]_D^{20} = -253°$ (CH_2Cl_2). The paramagnetic nature of the complex does not allow its NMR characterization.

Crystallography

Data collection for **1** was performed on an APEXII Bruker-AXS diffractometer equipped with a CCD camera. Structures were solved by direct methods using either the *SIR97* program,[1] and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*)[2] with the aid of the *WINGX* program.[3] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. Details are given in Table S3. CCDC 2044039.

Theoretical calculations

Theoretical calculations on the radical gold neutral complexes and radical anion nickel complexes (doublet state) were performed with Density Functional Theory using the Gaussian 09 Revision D.01 software[4] with the B3LYP functional (hybrid Becke-3 parameter exchange functional[5] and the Lee-Yang-Parr nonlocal correlation functional)[6] and the LANL2DZ basis set.[7] GaussView 5.0.9 (Gaussian Inc., Wallingford, CT, USA) was used to generate the figures. The butoxy group in the OC_4 ligand was modeled as a methoxy group. Cartesian coordinates for optimized complexes are reported in Tables S4-S9.

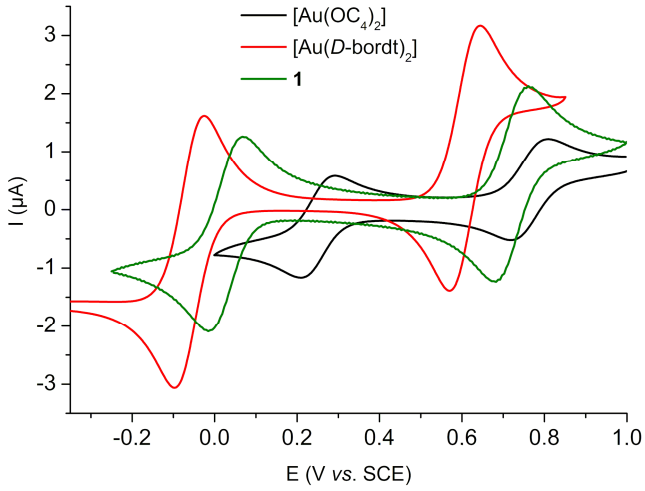


Fig. S1 Cyclic voltammetry of **1** and references complexes.

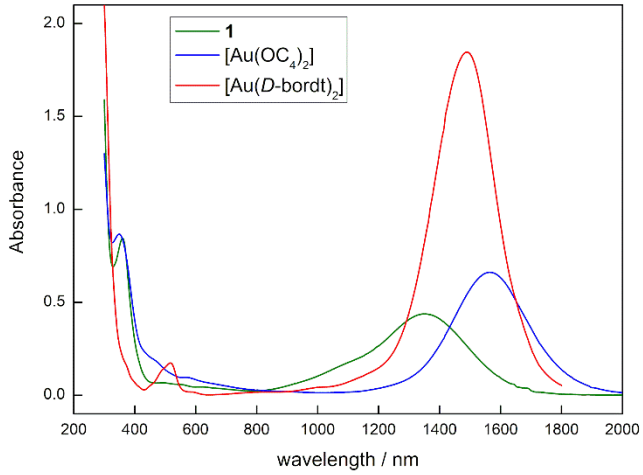


Fig. S2 UV-vis-NIR absorption of **1** and references complexes (in CH_2Cl_2, 10^{-4} M)

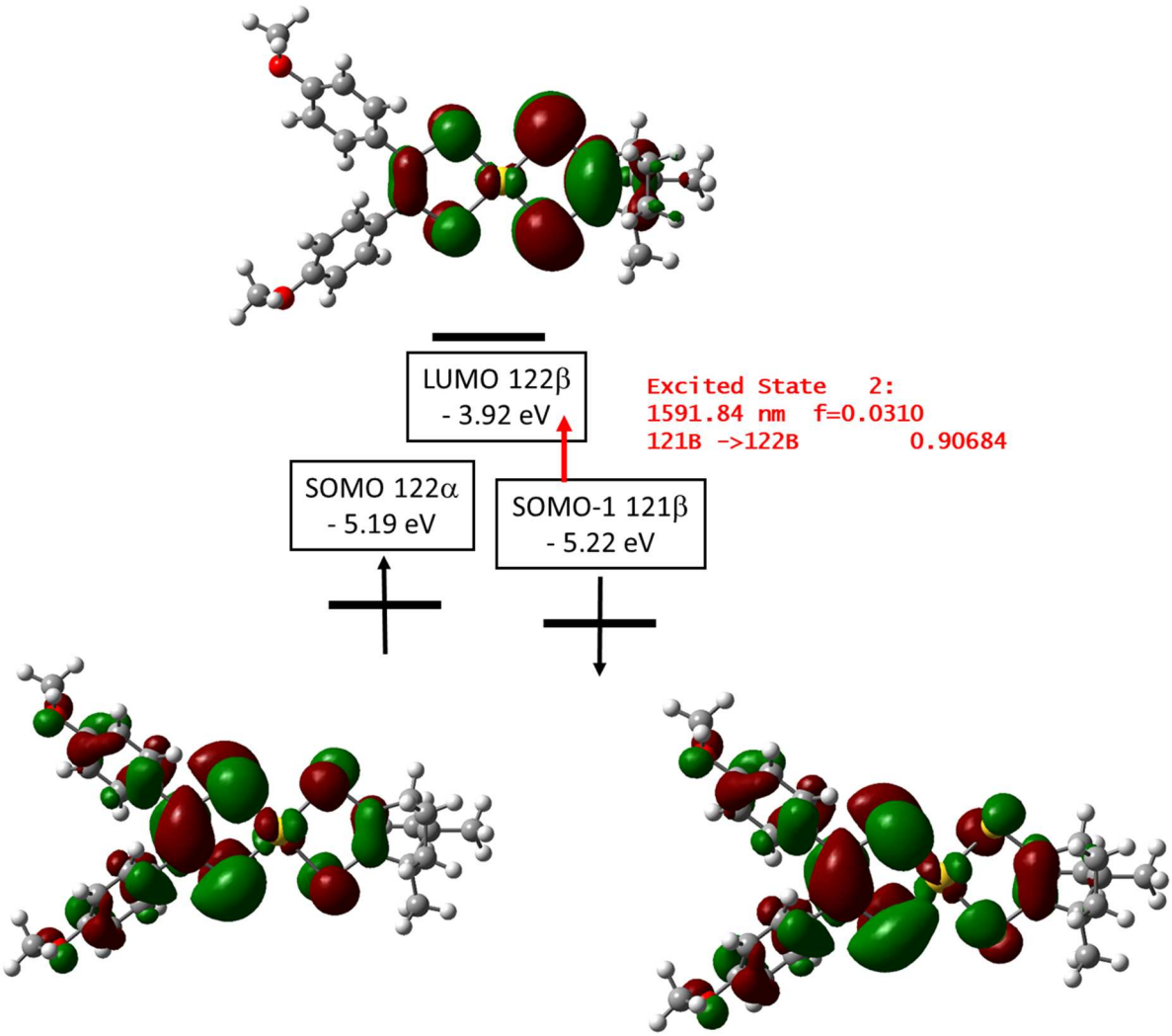


Fig. S3 Frontier molecular orbitals in the mixed ligand neutral radical complex **1** calculated by DFT shown with a cut-off of 0.04 [e/bohr^3]$^{1/2}$. The first significant low energy transition as calculated by TD DFT and assigned to a SOMO-1 to LUMO transition is shown in red.

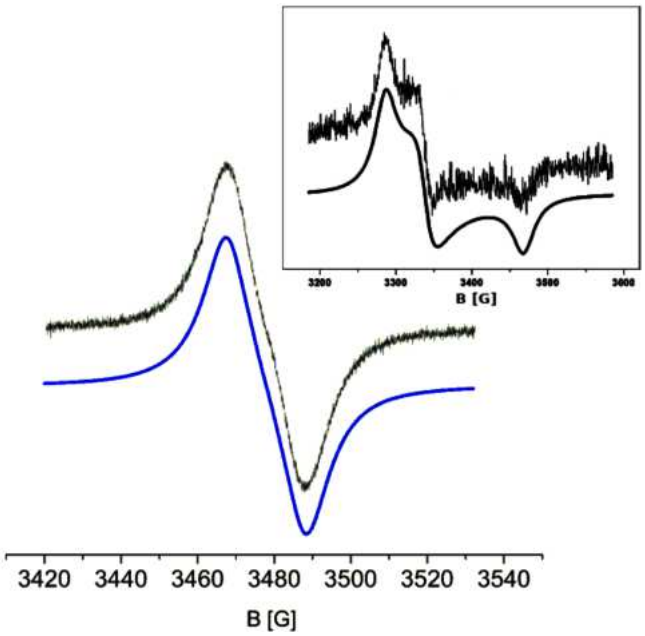


Fig. S4 Solution EPR (in CH_2Cl_2) of **1**. In insert: frozen solution spectrum (at 77 K).

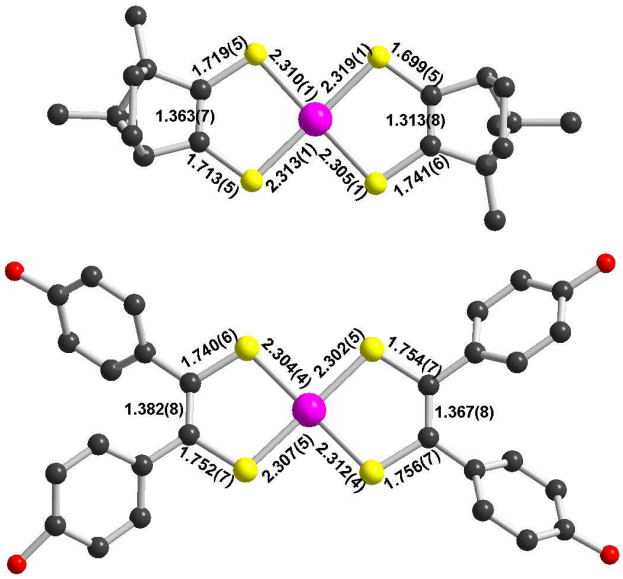


Fig. S5 Compared experimental bond distances (in Å) within the metallacycles in [Au(*D*-bordt)$_2$]$^{\bullet}$ (top) and [Au(OC$_4$)$_2$]$^{\bullet}$ (bottom). The butyl chains in [Au(OC$_4$)$_2$]$^{\bullet}$ and all hydrogen atoms have been removed for clarity

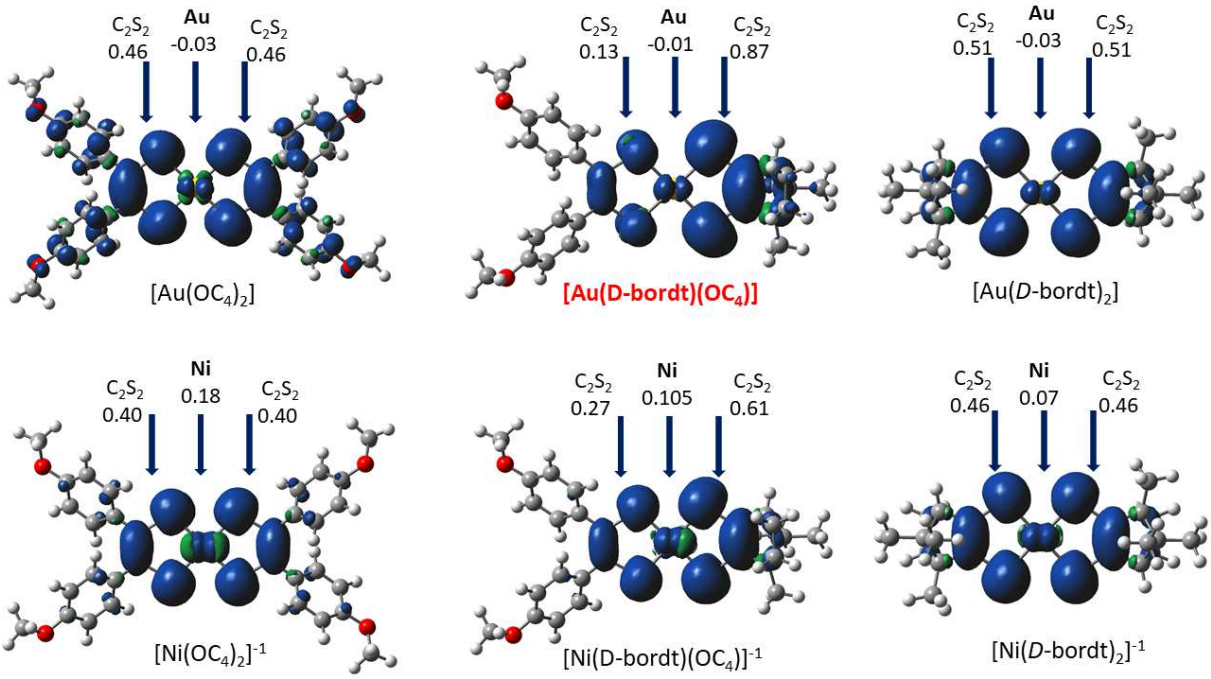


Fig. S6 Compared calculated spin densities in the metallacycles

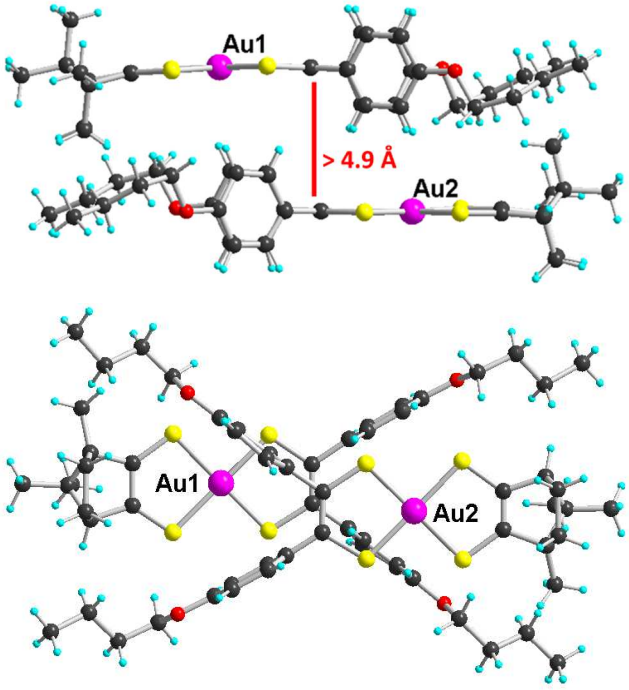


Fig. S7 Face-to-face association of **1** showing the large interplanar distance and strongly shifted overlap.

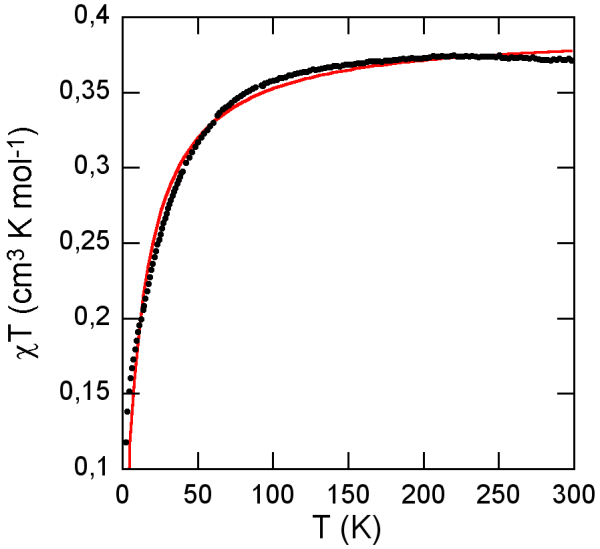
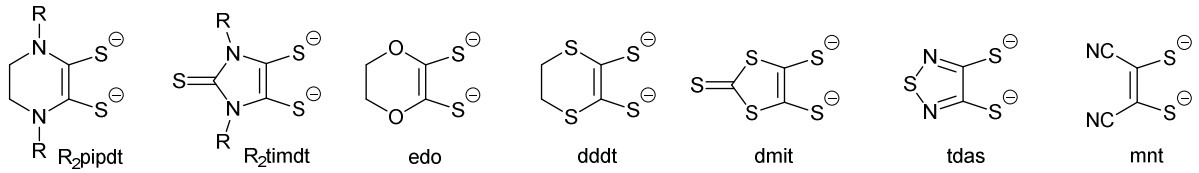


Fig. S8 Temperature dependence of the χ.T product for **1**. The solid line is a fit to the Curie-Weiss model.

Table S1. Comparison of $\Delta E = E_{1/2}(-1/0) - E_{1/2}(-2/-1)$ values for reported mixed-ligand bis(dithiolene) Ni complexes $[Ni(dt_{push})(dt_{pull})]^{-2,-1,0}$ with the push and pull dithiolene ligands and their symmetric precursors. ΔE values were calculated from reported $E_{1/2}$.[8,9,10]



[Ni(push)(pull)]	ΔE [Ni(push)$_2$]	ΔE [Ni(push)(pull)]	ΔE [Ni(pull)$_2$]	Ref
[Ni(^{i}Pr$_2$timdt)(mnt)]	0.50	0.66	0.84	8
[Ni(dmit)(mnt)]	0.425	0.67	0.84	8
[Ni(dddt)(mnt)]	0.75	0.77	0.84	8
[Ni(dmit)(dddt)]	0.425	0.61	0.75	8
[Ni(^{i}Pr$_2$pipdt)(dmit)]	0.32	0.57	0.425	9
[Ni(Me$_2$pipdt)(mnt)]	0.31	0.44	0.84	9
[Ni(Me$_2$pipdt)(tdas)]	0.31	0.45	0.62	9
[Ni(edo)(dddt)]	0.69	0.73	0.75	10
[Ni(edo)(dmit)]	0.69	0.73	0.56	10
[Ni(edo)(mnt)]	0.69	0.80	0.91	10

Table S2 Averaged, DFT-calculated bond distances (Å) within the NiS_2C_2 metallacycles in the mixed-ligand symmetric nickel complex [Ni(*D*-bordt)(OC$_4$)]$^{-1}$ and the two symmetric complexes [Ni(*D*-bordt)$_2$]$^{-1}$ and [Ni(OC$_4$)$_2$]$^{-1}$.

	D-bordt side			OC$_4$ side		
	Ni–S	S–C	C=C	Ni–S	S–C	C=C
[Ni(*D*-bordt)$_2$]$^{-1}$	*2.302*	*1.781*	*1.372*	–	–	–
[Ni(*D*-bordt)(OC$_4$)]$^{-1}$	*2.312*	*1.770*	*1.380*	*2.253*	*1.822*	*1.377*
[Ni(OC$_4$)$_2$]$^{-1}$	–	–	–	*2.256*	*1.814*	*1.382*

Table S3 Crystallographic data

Compound	**1**
Formulae	$C_{32}H_{40}AuO_2S_4$
FW ($g.mol^{-1}$)	781.85
System	triclinic
Space group	P1
a (Å)	10.7823(3)
b (Å)	11.0287(3)
c (Å)	15.3429(4)
α (deg)	107.822(4)
β (deg)	91.112(3)
γ (deg)	107.275(3)
V ($Å^3$)	1646.34(8)
T (K)	100(2)
Crystal size	0.4 × 0.3 × 0.2
Z	2
D_{calc} ($g.cm^{-1}$)	1.577
μ (mm^{-1})	4.748
Total refls	21867
Abs corr	multi-scan
T_{min}, T_{max}	0.197, 0.387
Uniq refls (R_{int})	13254 (0.0271)
Uniq refls (I > 2σ(I))	12219
R_1, wR_2	0.0301, 0.0683
R_1, wR_2 (all data)	0.0358, 0.0713
Flack param.	0.078(14)
GOF	1.021

Table S4 Cartesian coordinates for optimized neutral doublet [Au(*D*-bordt)(OC_4)]

(with methoxy instead of butoxy groups)

Au	1.17738368	0.07582111	-0.07111191
S	3.02595451	-1.62375387	-0.05185260
S	2.90574767	1.89150319	0.07791883
S	-0.64682731	1.67832178	0.10470363
S	-0.52339611	-1.64364252	-0.36123257
O	-6.86793979	3.83520661	-0.49223882
O	-6.51135539	-4.34225768	0.06991509
C	4.39334774	-0.52076826	0.07535704
C	4.33883766	0.87465221	0.14031900
C	5.76533628	1.36448462	0.36208995
C	6.57639318	0.30317272	-0.47985366
C	5.86557954	-0.93045645	0.24224309
C	6.16174460	-0.61072081	1.76469846
C	6.10317727	0.95301830	1.84310300
C	8.10601272	0.36949214	-0.27295479
C	6.30641568	0.38214568	-2.00048753
C	6.24648937	-2.34097716	-0.20004074
C	-2.14994074	0.64099077	-0.07533330
C	-3.38566834	1.46212667	-0.13976938
C	-4.34934497	1.25675494	-1.16447423
C	-5.49087575	2.05627035	-1.25108840
C	-5.69998088	3.09511751	-0.31532030
C	-4.75544476	3.32366744	0.70613010
C	-3.61180101	2.50944030	0.78311837
C	-7.13662107	4.94798339	0.40948120
C	-2.09909279	-0.72142989	-0.18505287
C	-3.27272933	-1.62911563	-0.11534216
C	-3.43736975	-2.68541494	-1.05065327
C	-4.51965830	-3.56700862	-0.96449475
C	-5.46976777	-3.41587571	0.06812339
C	-5.32364494	-2.37749004	1.01388070
C	-4.23119655	-1.50139596	0.91680773
C	-7.53221593	-4.24797552	1.10538438
H	5.93957376	2.41717867	0.12856192
H	5.42526200	-1.09296708	2.41580140
H	7.14937344	-0.99796823	2.04104597
H	7.06220028	1.38416434	2.15058080
H	5.33906961	1.31289715	2.53915803
H	8.49450328	1.31957683	-0.66433364
H	8.41937794	0.28975661	0.77175093
H	8.59987517	-0.43711777	-0.83065552
H	6.70517566	1.32139425	-2.40679454
H	6.81078716	-0.44130843	-2.52308662
H	5.24143609	0.33629140	-2.24937735
H	5.70036369	-3.09790012	0.37698283
H	6.01794587	-2.50743335	-1.25977316
H	7.31900767	-2.51608770	-0.04758464
H	-4.18632520	0.47237744	-1.89713089
H	-6.22768887	1.90705735	-2.03445112
H	-4.89626237	4.11488216	1.43539276
H	-2.89141170	2.68272532	1.57852287
H	-8.08138296	5.37406114	0.06656148
H	-6.34436171	5.70687743	0.35027395
H	-7.24137535	4.60250083	1.44737469
H	-2.71575809	-2.80349591	-1.85489874
H	-4.65247851	-4.37226956	-1.68033660
H	-6.03757342	-2.24857577	1.82121703
H	-4.11289689	-0.71434428	1.65559628
H	-8.22864134	-5.06242993	0.89708106
H	-8.06132661	-3.28628467	1.05554028
H	-7.09696458	-4.38000334	2.10558893

Table S5 Cartesian coordinates for optimized neutral doublet [$Au(OC_4)_2$]

(with methoxy instead of butoxy groups)

Au	-0.01603543	-0.02483517	-0.01239909
S	1.77921264	1.64192754	-0.06234781
S	1.74096522	-1.72762925	0.09193494
S	-1.80690731	-1.69667799	-0.02887489
S	-1.77928118	1.67626388	-0.03189171
O	7.95195779	3.80610359	0.95376612
O	-7.99455894	-3.83543429	0.93382174
O	-7.94742576	3.90497925	-0.94400680
C	3.28505476	0.63420958	0.05929223
C	4.51186810	1.45353870	0.24035201
C	4.74423802	2.60477259	-0.54716607
C	5.45506691	1.14058870	1.25747520
C	5.87609318	3.41465872	-0.34992237
C	6.58106285	1.93858653	1.46693060
C	6.79946499	3.07989618	0.66226480
C	8.22895261	5.01971610	0.19566983
C	3.27078789	-0.75131422	0.04665334
C	-3.30551414	0.69402006	-0.06552501
C	-4.52221769	1.52768594	-0.24573420
C	-4.71023622	2.71474718	0.49963644
C	-5.50306111	1.18877883	-1.21780252
C	-6.62258760	1.99642604	-1.42418821
C	-5.83549349	3.53410931	0.30590342
C	-6.79712269	3.17312340	-0.66078108
C	-3.31656162	-0.69008716	0.01112096
C	-4.54506242	-1.50462748	0.19959577
C	-5.51237775	-1.15107518	1.17993302
C	-4.75624882	-2.68958003	-0.54280071
C	-5.89060582	-3.49345513	-0.33749974
C	-6.64080649	-1.94317408	1.39772576
C	-6.83798756	-3.11863450	0.63794821
C	-8.25830739	-5.07437932	0.21254802
C	-8.19139864	5.14295757	-0.21417296
C	6.76428195	-3.26872859	-0.34162714
C	5.77801193	-3.56908023	0.62291585
C	4.65553480	-2.74638995	0.75200522
C	4.48737079	-1.59734879	-0.06643765
C	5.48380520	-1.31857000	-1.03143508
C	6.61337330	-2.13914624	-1.17535806
O	7.84243186	-4.14888605	-0.39314930
C	8.90160754	-3.90831718	-1.36502202
H	9.15941041	5.41151556	0.61079255
H	8.36385931	4.79920165	-0.87229395
H	7.42598201	5.75858445	0.32294777
H	-7.45987216	-5.80962508	0.38224411
H	-9.19813095	-5.44995701	0.62144120
H	-8.37047995	-4.89034932	-0.86482038
H	-9.13187034	5.52951786	-0.61116205
H	-8.29375629	4.95484521	0.86347270
H	-7.38775266	5.87133318	-0.38893891
H	4.03726051	2.86554231	-1.33042882
H	5.28762170	0.27648996	1.89262399
H	6.02337327	4.28624317	-0.97955003
H	7.29880675	1.70904987	2.24844632
H	-3.97446477	2.99493945	1.24888453
H	-5.37048237	0.29560521	-1.82011784
H	-7.37042338	1.74615886	-2.17029048
H	-5.94943181	4.43223103	0.90428130
H	-5.36186778	-0.25953244	1.78047106
H	-4.03104565	-2.98101874	-1.29807872
H	-6.02187961	-4.39082572	-0.93347093
H	-7.37795341	-1.68222270	2.15076400
H	5.91482578	-4.44275145	1.25246569
H	3.90369277	-2.98364693	1.49986350
H	5.36541814	-0.45966050	-1.68485018
H	7.35328602	-1.89646985	-1.93139254
H	9.38832757	-2.93895126	-1.19028462
H	8.51426027	-3.94936223	-2.39229890
H	9.62110407	-4.71459690	-1.21076158

Table S6 Cartesian coordinates for optimized neutral doublet [Au(*D*-bordt)$_2$]

Au	0.00001486	-0.00003287	-0.10352611
S	1.62911134	-1.84549821	-0.10200039
S	1.83579008	1.64033622	-0.08132541
S	-1.62910079	1.84545379	-0.10200293
S	-1.83582941	-1.64035433	-0.08126038
C	3.12253580	-0.87122759	-0.04559190
C	4.54623447	-1.41757841	-0.10919716
C	5.04153879	-1.08957233	-1.56751848
C	5.13511088	0.47486240	-1.55872114
C	4.70000208	0.87634009	-0.09034203
C	3.20911568	0.49834875	-0.03761181
C	5.30742545	-0.33588278	0.75656215
C	4.89851626	-0.33370461	2.24799049
C	6.84770696	-0.44878588	0.69651884
C	5.07332813	2.29868380	0.32193242
C	-3.12251832	0.87122688	-0.04557029
C	-4.54619505	1.41760558	-0.10917277
C	-5.04156159	1.08965052	-1.56747461
C	-5.13497279	-0.47479678	-1.55877487
C	-4.70000989	-0.87631041	-0.09034283
C	-3.20911713	-0.49835914	-0.03755178
C	-5.30743566	0.33587751	0.75654853
C	-4.89857520	0.33375817	2.24798390
C	-6.84771564	0.44888919	0.69643503
C	-5.07345823	-2.29862849	0.32190912
H	4.66772074	-2.46117453	0.19195377
H	4.33851412	-1.46539886	-2.31745787
H	6.01428084	-1.55640060	-1.75923154
H	6.15476385	0.82476756	-1.75955462
H	4.47536114	0.93959761	-2.29888651
H	5.24055768	-1.25757305	2.73405182
H	3.81678140	-0.25845502	2.39222961
H	5.37053735	0.50664312	2.77440056
H	7.31142842	0.37029253	1.26212834
H	7.25546290	-0.42474101	-0.31742463
H	7.17081094	-1.38916009	1.16377014
H	4.60867723	3.03916770	-0.34207479
H	6.16001249	2.44318380	0.26927114
H	4.74663682	2.52220163	1.34496068
H	-4.66769872	2.46118520	0.19203097
H	-4.33866713	1.46559766	-2.31746600
H	-6.01439096	1.55637023	-1.75902067
H	-6.15454747	-0.82480378	-1.75981205
H	-4.47504408	-0.93941651	-2.29886170
H	-3.81680857	0.25905964	2.39225240
H	-5.37017973	-0.50685764	2.77432200
H	-5.24111934	1.25741801	2.73409984
H	-7.31151494	-0.36960156	1.26280088
H	-7.25549343	0.42392226	-0.31748287
H	-7.17069939	1.38974035	1.16282379
H	-4.60834071	-3.03919900	-0.34166876
H	-6.16010240	-2.44320375	0.26859316
H	-4.74738279	-2.52194370	1.34517641

Table S7 Cartesian coordinates for optimized monoanionic doublet [Ni(*D*-bordt)(OC_4)]$^{-1}$

(with methoxy instead of butoxy groups)

Ni	1.36409578	0.08898987	-0.08255991
S	3.02102864	-1.52303527	-0.12497410
S	2.88939930	1.81487304	0.11690327
S	-0.28172725	1.62460692	-0.01063634
S	-0.15710774	-1.56573085	-0.25279536
O	-6.60176675	3.82016663	-0.46680402
O	-6.21202289	-4.34599015	0.05709666
C	4.45271280	-0.49020627	0.02659135
C	4.39494746	0.88494172	0.12378005
C	5.81970538	1.37951983	0.36819445
C	6.64644609	0.33795726	-0.48225334
C	5.92372977	-0.90809149	0.20391588
C	6.21600066	-0.62362227	1.73283731
C	6.15416556	0.94068233	1.84287618
C	8.17620332	0.39966815	-0.25873915
C	6.39754968	0.44815218	-2.00439045
C	6.30552518	-2.30880671	-0.26806852
C	-1.82266056	0.65575054	-0.10382276
C	-3.06849683	1.47186195	-0.16439081
C	-4.09222645	1.20209969	-1.11203335
C	-5.24622941	1.99191240	-1.18659997
C	-5.40824054	3.08670915	-0.31377876
C	-4.40405476	3.38835226	0.62619171
C	-3.24982174	2.58415035	0.68843267
C	-6.80115598	4.97944999	0.38291462
C	-1.76793676	-0.71830250	-0.17358914
C	-2.94613937	-1.62841023	-0.10449187
C	-3.06329261	-2.74033823	-0.97924287
C	-4.15217165	-3.61892588	-0.90496072
C	-5.15770852	-3.41163599	0.06021324
C	-5.05996263	-2.32653617	0.95308430
C	-3.95974710	-1.45339823	0.86510068
C	-7.27011815	-4.18020310	1.03604601
H	5.99702146	2.43776692	0.15545739
H	5.46538052	-1.11614653	2.36028573
H	7.20163086	-1.01510535	2.02130750
H	7.11010929	1.36434237	2.17908838
H	5.37485274	1.28144833	2.53216655
H	8.57106845	1.35606500	-0.63183047
H	8.47438454	0.30489479	0.78979171
H	8.67656115	-0.40169200	-0.82101365
H	6.80291332	1.39597827	-2.38789038
H	6.90418070	-0.36853747	-2.53891623
H	5.33342154	0.41003841	-2.25253665
H	5.72260421	-3.06857239	0.26829653
H	6.09780718	-2.43940108	-1.33771549
H	7.37215929	-2.51014933	-0.09272716
H	-3.96882884	0.37085084	-1.79931522
H	-6.02477193	1.78454097	-1.91553883
H	-4.49982822	4.23258847	1.30288282
H	-2.46973160	2.82364802	1.40570189
H	-7.76875774	5.39465878	0.08905418
H	-6.01428576	5.73230795	0.22789286
H	-6.82826906	4.69987646	1.44670201
H	-2.28391605	-2.90913099	-1.71705024
H	-4.24050509	-4.46688859	-1.57843698
H	-5.81489272	-2.15182066	1.71433863
H	-3.88149592	-0.62670881	1.56482685
H	-7.97088588	-4.99850843	0.85083188
H	-7.78684491	-3.21704040	0.91155833
H	-6.88307050	-4.25223724	2.06326418

Table S8 Cartesian coordinates for optimized monoanionic doublet $[Ni(OC_4)_2]^{-1}$

(with methoxy instead of butoxy groups)

Ni	0.02285425	-0.03451997	-0.03133329
S	-1.58178444	1.55186582	-0.05030468
S	-1.54768904	-1.65479569	-0.05575204
S	1.62712946	-1.62029401	-0.06949921
S	1.59441800	1.58326068	0.04597535
O	-7.82705333	3.85430619	-0.83286674
O	7.87892789	-3.90534747	-0.81550681
O	7.78929680	3.98397111	0.91661732
C	-3.14009666	0.62251065	-0.09385467
C	-4.36471192	1.45946551	-0.24618398
C	-4.54016346	2.63853614	0.51226152
C	-5.36899120	1.13831975	-1.19841348
C	-5.67222802	3.46113995	0.35494630
C	-6.49981361	1.94604095	-1.36756580
C	-6.65770386	3.10965285	-0.58773039
C	-8.01945594	5.08643560	-0.09002245
C	-3.12502346	-0.75889790	-0.05774131
C	3.17174174	0.68631399	0.05079363
C	4.37869896	1.54199058	0.23475377
C	4.53007087	2.75193082	-0.47890847
C	5.38892927	1.20573998	1.17520637
C	6.50249749	2.02976527	1.37637486
C	5.64488839	3.59092947	-0.28947332
C	6.63660180	3.22494166	0.64118351
C	3.18608950	-0.69275095	-0.04008967
C	4.41259679	-1.52539519	-0.19924030
C	5.43449657	-1.17053303	-1.11999063
C	4.57220053	-2.73240875	0.51750859
C	5.70538367	-3.55109231	0.34956808
C	6.56648264	-1.97418553	-1.29958378
C	6.70793918	-3.16705303	-0.56200993
C	8.06339686	-5.15782630	-0.10528555
C	7.96853972	5.23600217	0.20433159
C	-6.60623306	-3.31363798	0.32813344
C	-5.59408277	-3.62874788	-0.60051056
C	-4.47539001	-2.79499137	-0.72415904
C	-4.33462767	-1.62221647	0.06293632
C	-5.35570716	-1.33751525	0.99785835
C	-6.48530611	-2.16545860	1.13534008
O	-7.68975687	-4.21044053	0.37840069
C	-8.75936781	-3.93588932	1.32035493
H	-3.77378770	2.91670196	1.23039885
H	-5.24827832	0.25349815	-1.81568749
H	-5.76573734	4.35744790	0.96118918
H	-7.26316126	1.70049939	-2.10055786
H	-8.96786053	5.49706474	-0.44589185
H	-8.08227907	4.89893843	0.99219424
H	-7.20974701	5.80457509	-0.28589087
H	3.75908774	3.04032307	-1.18801964
H	5.28667343	0.29520304	1.75749544
H	7.27159069	1.77185946	2.09898890
H	5.72103525	4.51026841	-0.86271323
H	5.32663215	-0.26221292	-1.70472261
H	3.79291378	-3.03521078	1.21137927
H	5.78684262	-4.46922755	0.92399469
H	7.34428255	-1.70251034	-2.00768828
H	7.25890260	-5.87211763	-0.33405257
H	9.01827847	-5.55571705	-0.45821175
H	8.10924784	-5.00083499	0.98254500
H	8.91027826	5.64989663	0.57379559
H	8.03780124	5.07496413	-0.88166538
H	7.14910970	5.93909930	0.41412791
H	-5.70137732	-4.52334958	-1.20740517
H	-3.69189158	-3.04691694	-1.43323689
H	-5.26037971	-0.46098819	1.63163916
H	-7.24489624	-1.90808723	1.86779122
H	-9.24161233	-2.96967631	1.11107907
H	-8.39303105	-3.94038940	2.35752524
H	-9.48296283	-4.74373774	1.18433748

Table S9 Cartesian coordinates for optimized monoanionic doublet [Ni(*D*-bordt)$_2$]$^{-1}$

Ni	0.00000868	-0.00000689	-0.13342301
S	1.47871325	-1.76392878	-0.13280025
S	1.68207851	1.57158938	-0.11843864
S	-1.47869463	1.76389775	-0.13277030
S	-1.68209555	-1.57158558	-0.11838458
C	3.01591884	-0.87055817	-0.06485541
C	4.44194097	-1.41620106	-0.12574421
C	4.94801807	-1.08975602	-1.58114186
C	5.04363564	0.47689136	-1.57028065
C	4.59588244	0.87320747	-0.10477521
C	3.10334634	0.49836069	-0.05622317
C	5.20598055	-0.33728758	0.73815158
C	4.79466317	-0.33763191	2.22891365
C	6.74885876	-0.44914892	0.68369058
C	4.96701673	2.29471993	0.31158686
C	-3.01591384	0.87055684	-0.06479953
C	-4.44191350	1.41622676	-0.12560398
C	-4.94806897	1.08995884	-1.58099526
C	-5.04348390	-0.47670020	-1.57037310
C	-4.59587987	-0.87318122	-0.10484462
C	-3.10334005	-0.49836564	-0.05614898
C	-5.20599993	0.33719854	0.73818298
C	-4.79471242	0.33741423	2.22894969
C	-6.74887469	0.44913391	0.68368419
C	-4.96708241	-2.29474663	0.31127777
H	4.56465201	-2.46084962	0.17611456
H	4.23701616	-1.46018479	-2.32674759
H	5.92208075	-1.55669829	-1.78200738
H	6.06552774	0.82593171	-1.77682673
H	4.37753715	0.94069225	-2.30583699
H	5.13248079	-1.26473954	2.71539118
H	3.71156028	-0.26250277	2.35528882
H	5.26302931	0.50383814	2.76023802
H	7.21175810	0.37659848	1.24302490
H	7.15448482	-0.43148945	-0.33203195
H	7.07324130	-1.38746095	1.15742131
H	4.46348772	3.02884265	-0.33080454
H	6.05150459	2.46113645	0.23529428
H	4.65422604	2.50164808	1.34291675
H	-4.56463590	2.46082804	0.17641062
H	-4.23719583	1.46058898	-2.32662011
H	-5.92222220	1.55679784	-1.78167141
H	-6.06529813	-0.82583543	-1.77711748
H	-4.37721416	-0.94030752	-2.30589926
H	-3.71157256	0.26285909	2.35531807
H	-5.26258373	-0.50445470	2.76006972
H	-5.13308728	1.26420166	2.71565673
H	-7.21181525	-0.37615042	1.24365787
H	-7.15453896	0.43071739	-0.33200898
H	-7.07316927	1.38782712	1.15671844
H	-4.46338441	-3.02878202	-0.33107562
H	-6.05154931	-2.46117230	0.23470609
H	-4.65453965	-2.50179874	1.34265741

References

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *J. Appl. Cryst.*, 1999, **32**, 115–119.

[2] G. M. Sheldrick, *Acta Crystallogr.,* 2008, **A64**, 112–122.

[3] L. J. Farrugia, *J. Appl. Cryst.*, 2012, **45**, 849–854.

[4] Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[5] (a) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098. (b) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 1372. (c) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.

[6] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

[7] (a) W. R. Wadt, P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284. (b) P. J. Hay, W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.

[8] P. Deplano, L. Pilia, D. Espa, M. L. Mercuri and A. Serpe, *Coord. Chem. Rev.*, 2010, **254**, 1434–1447.

[9] B. Mogesa, E. Perera, H. M. Rhoda, J. K. Gibson, J. Oomens, G. Berden, M. J. van Stipdonk, V. N. Nemykin and P. Basu, *Inorg. Chem.*, 2015, **54**, 7703–7716.

[10] E. Watanabe, M. Fujiwara, J.-I. Yamaura and R. Kato, *J. Mater. Chem.*, 2001, **11**, 2131–2141.