

Supplementary Information

Theoretical Study on Charge Transport of Dithiolene Nickel Complexes

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Supplementary information contains *i*) shapes of molecules **1a-3a** and **1b-3b** at neutral, anionic and cationic states (Fig. S1) and *ii*) XYZ-coordinates of the molecules obtained at the PBE/6-31G(d,p) level of theory (Table S1).

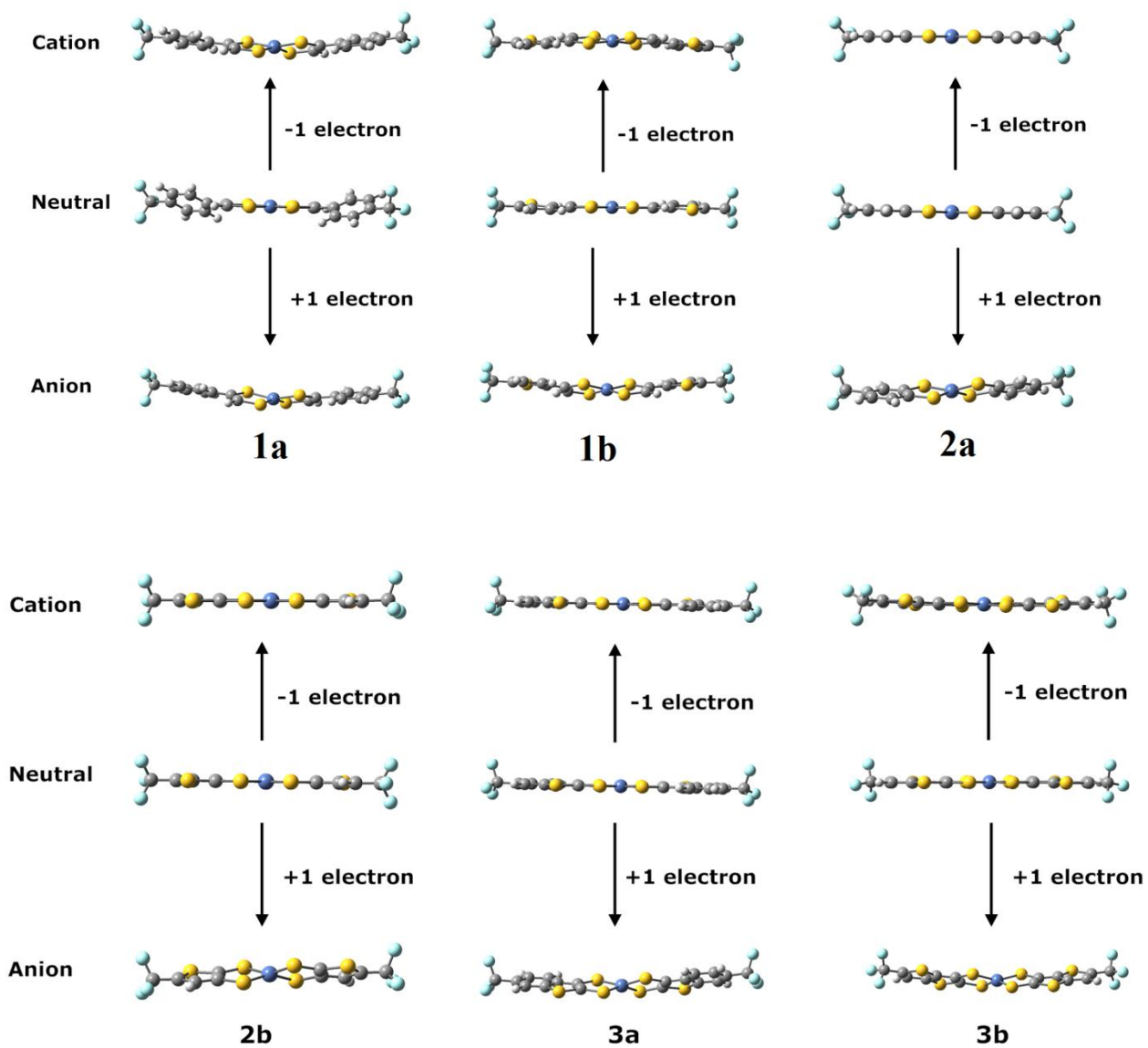


Fig. S1 Shapes of molecules **1a-3a** and **1b-3b** at neutral, anionic and cationic states obtained at the PBE/6-31G(d,p) level of theory

Table S1. Total energy (a.u.) and differences in energy (a.u) of compounds **1a-3a** and **1b-3b** at neutral state obtained from PBE/6-31G(d,p) level of theory

	E(CS)	E(CSBS)	E(OS)	$\Delta E(\text{CS-CSBS})$	$\Delta E(\text{CS-OS})$
1a	-4389.615099	-4389.615099	-4389.615099	0.00000	0.00000
1b	-5030.968974	-5030.968974	-5030.968974	0.00000	0.00000
2a	-4234.991936	-4234.991962	-4234.99196	0.00003	0.00002
2b	-4876.340695	-4876.340695	-4876.340695	0.00000	0.00000
3a	-5183.278631	-5183.278631	-5183.278631	0.00000	0.00000
3b	-5824.613895	-5824.613895	-5824.613896	0.00000	0.00000

Table S2. Total energy (a.u.) and differences in energy (a.u) of compounds **1a-3a** and **1b-3b** at neutral state obtained from B3LYP/6-31G(d,p) level of theory

	E(CS)	E(CSBS)	E(OS)	$\Delta E(\text{CS-CSBS})$	$\Delta E(\text{CS-OS})$
1a	-4391.9900	-4391.9900	-4391.9900442	0.00000	0.00000
1b	-5033.489815	-5033.489815	-5033.4898154	0.00000	0.00000
2a	-4237.1588	-4237.1593	-4237.1593045	0.00050	0.00050
2b	-4878.6585	-4878.6585	-4878.6585224	0.00000	0.00000
3a	-5185.9821	-5185.9821	-5185.9821099	0.00000	0.00001
3b	-5827.4646	-5827.4646	-5827.4646150	0.00000	0.00000

CS: Closed shell singlet state

CSBS: Closed shell singlet – broken symmetry by applying “stable=opt” for single point calculations

OS: Open shell singlet state by using keyword guess=mix for optimization

Table S2 the XYZ-coordinates of the molecules obtained at the PBE/6-31G(d,p) level of theory

Compound 1a				
28	0.001401000	0.013318000	-0.057608000	
16	0.742905000	2.015556000	-0.085314000	
16	-1.972954000	0.821519000	0.013369000	
16	1.975905000	-0.796191000	-0.019339000	
16	-0.739520000	-1.988854000	-0.100907000	
6	-3.029538000	-0.557370000	-0.008183000	
6	-2.438936000	-1.815059000	-0.059652000	
6	2.442709000	1.840653000	-0.066103000	
6	3.033249000	0.582255000	-0.036416000	
6	4.492093000	0.373619000	-0.021952000	
6	-4.488503000	-0.351704000	0.023395000	
6	5.355690000	1.337811000	0.549746000	
6	5.065739000	-0.792296000	-0.578708000	
6	-5.343291000	-1.321197000	0.599244000	
6	-5.070470000	0.818837000	-0.514713000	
1	4.936396000	2.232315000	1.018036000	
1	4.415334000	-1.539608000	-1.041083000	
1	-4.425882000	1.575938000	-0.969309000	
1	-4.915841000	-2.213603000	1.064159000	
6	6.738001000	1.146018000	0.558836000	
6	6.447703000	-0.987102000	-0.567198000	
6	-6.452875000	1.008861000	-0.489272000	
6	-6.726074000	-1.133750000	0.623148000	
1	6.880032000	-1.885777000	-1.013536000	
1	-7.374501000	-1.882671000	1.084396000	
6	7.290264000	-0.017836000	-0.000098000	
6	-7.287235000	0.031774000	0.076789000	
1	7.394546000	1.898590000	1.002382000	
1	-6.890572000	1.917926000	-0.908628000	
6	8.778654000	-0.252201000	0.069005000	
6	-8.785328000	0.203903000	0.045891000	
9	9.475573000	0.915395000	-0.000008000	
9	9.211351000	-1.053329000	-0.942097000	
9	9.131704000	-0.857539000	1.238282000	
9	-9.383670000	-0.403954000	1.106820000	
9	-9.143865000	1.516277000	0.064049000	
9	-9.323807000	-0.341965000	-1.081587000	
1	3.035016000	2.759101000	-0.121108000	
1	-3.031809000	-2.732901000	-0.118880000	
Compound 1b				
28	0.000000000	0.000000000	0.000000000	
16	1.849508000	1.070352000	-0.034573000	
16	-1.001340000	1.883751000	-0.067070000	
16	1.001340000	-1.883751000	0.067068000	
16	-1.849508000	-1.070352000	0.034573000	
6	-2.659881000	1.486975000	-0.070227000	

6	-3.080953000	0.159537000	-0.026649000
6	3.080953000	-0.159537000	0.026648000
6	2.659881000	-1.486975000	0.070226000
6	4.475014000	0.245524000	0.030981000
6	-4.475014000	-0.245524000	-0.030982000
6	5.001474000	1.533326000	0.099942000
6	-5.001474000	-1.533326000	-0.099944000
1	3.366933000	-2.322454000	0.117107000
1	4.368869000	2.419841000	0.168532000
1	-4.368869000	-2.419841000	-0.168536000
1	-3.366933000	2.322454000	-0.117109000
6	6.977459000	0.305508000	-0.013845000
6	6.417028000	1.565826000	0.076420000
6	-6.417028000	-1.565826000	-0.076422000
6	-6.977459000	-0.305508000	0.013845000
1	7.018671000	2.474260000	0.123584000
1	-7.018671000	-2.474259000	-0.123587000
16	5.769659000	-0.942154000	-0.074075000
16	-5.769659000	0.942154000	0.074076000
6	-8.433932000	0.037538000	0.012205000
6	8.433932000	-0.037538000	-0.012204000
9	-9.183783000	-1.076177000	0.213254000
9	-8.739061000	0.937678000	0.987027000
9	-8.826023000	0.590950000	-1.168974000
9	8.826023000	-0.590950000	1.168976000
9	8.739062000	-0.937679000	-0.987025000
9	9.183783000	1.076177000	-0.213253000
Compound 2a			
28	0.000000000	0.000000000	-0.047443000
16	1.694854000	-1.300851000	-0.038540000
16	-1.215800000	-1.761745000	-0.045137000
16	1.215799000	1.761744000	-0.045137000
16	-1.694854000	1.300850000	-0.038538000
6	-2.847542000	-1.171776000	-0.027315000
6	-3.067375000	0.237807000	-0.023177000
6	3.067375000	-0.237807000	-0.023179000
6	2.847542000	1.171776000	-0.027315000
6	-4.388848000	0.745114000	-0.006293000
1	4.562248000	-1.823470000	-0.003969000
6	5.459754000	0.138887000	0.004606000
6	-5.459753000	-0.138886000	0.004610000
6	4.388848000	-0.745114000	-0.006296000
1	-4.562247000	1.823470000	-0.003965000
6	3.957176000	2.055021000	-0.018044000
1	3.785236000	3.134639000	-0.025037000
6	5.245081000	1.543847000	-0.002410000
1	6.105159000	2.218070000	-0.001071000
6	-3.957176000	-2.055021000	-0.018042000
1	-3.785237000	-3.134639000	-0.025036000
6	-5.245081000	-1.543847000	-0.002407000

1	-6.105159000	-2.218070000	-0.001066000
6	6.878189000	-0.373623000	0.057424000
6	-6.878188000	0.373624000	0.057424000
9	-7.454306000	0.093621000	1.259798000
9	-7.649913000	-0.218208000	-0.896305000
9	-6.947634000	1.716912000	-0.127460000
9	7.454291000	-0.093650000	1.259813000
9	6.947637000	-1.716907000	-0.127491000
9	7.649925000	0.218233000	-0.896280000
Compound 2b			
28	0.000000000	0.000000000	-0.000002000
16	-1.507972000	1.531555000	-0.000014000
16	1.427009000	1.611127000	-0.000018000
16	-1.427009000	-1.611127000	0.000014000
16	1.507972000	-1.531554000	0.000011000
6	2.923112000	0.776582000	-0.000011000
6	2.982197000	-0.634153000	0.000002000
6	-2.982197000	0.634153000	-0.000003000
6	-2.923112000	-0.776582000	0.000009000
6	4.322308000	-1.129551000	0.000006000
1	-4.596274000	2.184589000	-0.000014000
16	4.521742000	1.492461000	-0.000018000
6	-5.245375000	0.113235000	0.000005000
6	5.245375000	-0.113235000	-0.000003000
16	-4.521742000	-1.492461000	0.000018000
6	-4.322308000	1.129551000	-0.000006000
1	4.596274000	-2.184589000	0.000016000
6	6.737756000	-0.257746000	-0.000001000
6	-6.737756000	0.257745000	0.000005000
9	7.295379000	0.329163000	1.092580000
9	7.088443000	-1.567318000	0.000004000
9	7.295382000	0.329156000	-1.092583000
9	-7.295381000	-0.329167000	-1.092572000
9	-7.295379000	-0.329154000	1.092590000
9	-7.088443000	1.567317000	-0.000002000
Compound 3a			
28	0.000077000	0.000091000	-0.017119000
16	1.772902000	-1.207828000	-0.017083000
16	-1.097141000	-1.856102000	-0.017134000
16	1.097213000	1.856296000	-0.017128000
16	-1.772885000	1.207782000	-0.017093000
6	-2.725478000	-1.323284000	-0.017230000
6	-3.044449000	0.047184000	-0.016400000
6	3.044435000	-0.047172000	-0.016378000
6	2.725489000	1.323323000	-0.017237000
6	-4.465586000	0.290214000	-0.014906000
16	-4.149540000	-2.354324000	-0.017709000
6	5.202806000	0.928242000	-0.014629000
6	-5.202809000	-0.928274000	-0.014625000

16	4.149572000	2.354318000	-0.017710000
6	4.465569000	-0.290217000	-0.014886000
6	-6.599992000	-0.942238000	-0.015162000
6	-5.168175000	1.513468000	-0.017512000
6	5.168124000	-1.513468000	-0.017510000
6	6.599993000	0.942225000	-0.015085000
1	-4.613904000	2.456078000	-0.022621000
1	7.165021000	1.876577000	-0.020368000
6	-7.271729000	0.288027000	-0.016387000
6	-6.561159000	1.508135000	-0.018188000
6	6.561100000	-1.508149000	-0.018175000
6	7.271685000	-0.288023000	-0.016320000
1	-7.164972000	-1.876615000	-0.020469000
1	-7.114752000	2.449874000	-0.028469000
1	4.613827000	-2.456039000	-0.022626000
6	-8.780002000	0.317556000	0.038765000
9	-9.327139000	-0.871252000	-0.332835000
9	-9.288330000	1.281174000	-0.777001000
9	-9.223556000	0.590628000	1.297818000
1	7.114687000	-2.449882000	-0.028437000
6	8.779923000	-0.317624000	0.038752000
9	9.327106000	0.871362000	-0.332029000
9	9.288136000	-1.280724000	-0.777721000
9	9.223507000	-0.591672000	1.297625000
Compound 3b			
28	0.000000000	0.000001000	0.004791000
16	1.861296000	-1.083066000	-0.003632000
16	-0.955484000	-1.926075000	0.011866000
16	0.955485000	1.926073000	0.012663000
16	-1.861295000	1.083070000	-0.003310000
6	-2.619361000	-1.524364000	0.005025000
6	-3.040914000	-0.173185000	-0.001317000
6	3.040915000	0.173187000	-0.001100000
6	2.619363000	1.524364000	0.005742000
6	-4.462008000	-0.089941000	-0.003791000
16	-3.957364000	-2.674804000	0.005787000
6	5.105145000	1.337320000	-0.000924000
6	-5.105142000	-1.337319000	-0.001686000
16	3.957367000	2.674803000	0.007006000
6	4.462009000	0.089943000	-0.003536000
1	-7.212255000	-2.098016000	-0.014291000
1	7.212257000	2.098020000	-0.013158000
16	5.612924000	-1.216502000	-0.025358000
16	-5.612924000	1.216511000	-0.025146000
6	6.519434000	1.256726000	-0.012851000
6	6.933340000	-0.062952000	-0.026089000
6	-6.519432000	-1.256722000	-0.013632000
6	-6.933339000	0.062960000	-0.026373000
6	-8.350197000	0.547770000	0.002146000
6	8.350194000	-0.547775000	0.002379000

9	9.208665000	0.484286000	-0.200176000
9	8.666261000	-1.122062000	1.195296000
9	8.577359000	-1.485039000	-0.957498000
9	-8.666236000	1.122008000	1.195094000
9	-9.208661000	-0.484291000	-0.200437000
9	-8.577401000	1.485069000	-0.957687000