Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Material

for

Tp*Cu(I)-CN-SiL$_2$-NC-Cu(I)Tp* – A hexacoordinate Si-complex as connector for redox active metals *via* π-conjugated ligands

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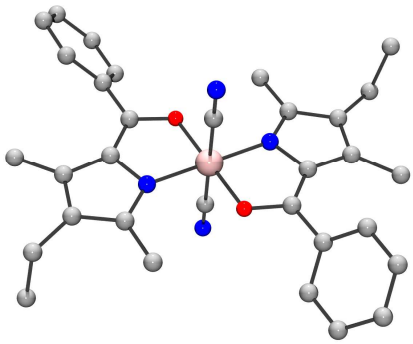

Figure SI1 Molecular structure of *all trans* $\mathbf{2}^{CN}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI1 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *all trans* $\mathbf{2}^{CN}$ (71 atoms), E = -1897.75214634 Hartree.

C	-5.8683	-3.25234	-0.229
C	-4.86402	-3.46965	0.70859
C	-5.79982	-2.15707	-1.0811
C	-3.79118	-2.59659	0.79278
C	-4.73905	-1.2674	-0.98643
C	-3.733	-1.47902	-0.0434
C	-2.57531	-0.58138	0.04222
O	-1.40815	-1.14399	0.10798
C	-2.59369	0.80581	0.07007
N	-1.31321	1.35635	0.10577
C	-3.55124	1.85027	0.16232
C	-1.43715	2.67814	0.1946
C	-2.81764	3.02676	0.23374
C	-5.03652	1.73481	0.22625
C	-3.3552	4.42043	0.32329
C	-3.54511	5.08515	-1.04249
C	-0.28243	3.60957	0.27363
C	5.86817	3.25234	-0.22896
C	4.86392	3.4696	0.70868
C	5.79966	2.15712	-1.08112
C	3.79107	2.59654	0.79285
C	4.73889	1.26746	-0.98646
C	3.73286	1.47903	-0.0434
C	2.57517	0.58138	0.04219
O	1.408	1.14395	0.10796
Si	-0.00005	-0.00004	0.10954
C	2.59361	-0.8058	0.07001
N	1.31315	-1.35642	0.10565
C	3.55121	-1.8502	0.16231
C	1.43719	-2.67821	0.19447
C	2.81769	-3.02673	0.23369
C	5.03648	-1.73465	0.22628
C	3.35533	-4.42037	0.32329
C	3.54596	-5.08488	-1.04249
C	0.28257	-3.60976	0.27355
H	-6.70053	-3.94244	-0.30052
H	-4.91569	-4.32477	1.37154
H	-6.56965	-1.99868	-1.82651
H	-2.99991	-2.75879	1.51354
H	-4.66598	-0.42752	-1.66554
H	-5.45811	2.56251	0.79889

H	-5.48938	1.76856	-0.76916
H	-5.35052	0.80322	0.69634
H	-4.31215	4.40479	0.85248
H	-2.68922	5.03224	0.93838
H	-3.94091	6.09784	-0.93487
H	-2.59954	5.14731	-1.58573
H	-4.23969	4.51336	-1.66149
H	0.22186	3.50862	1.2382
H	0.45361	3.3871	-0.49781
H	-0.61415	4.64103	0.16511
H	6.7004	3.94244	-0.30046
H	4.91562	4.32468	1.37168
H	6.56947	1.99877	-1.82655
H	2.99984	2.75871	1.51365
H	4.6658	0.4276	-1.66561
H	5.4581	-2.56232	0.79896
H	5.48939	-1.7684	-0.76911
H	5.35042	-0.80303	0.69637
H	4.31203	-4.40472	0.85294
H	2.68911	-5.03232	0.93797
H	3.94177	-6.09756	-0.93483
H	2.60065	-5.14702	-1.5862
H	4.2408	-4.51296	-1.66107
H	-0.22028	-3.51048	1.23906
H	-0.45458	-3.38599	-0.49642
H	0.61414	-4.64105	0.16286
C	-0.0001	-0.00001	-1.81555
C	0.	-0.0001	2.0349
N	-0.00012	0.00003	-2.97123
N	0.00005	-0.00014	3.19081

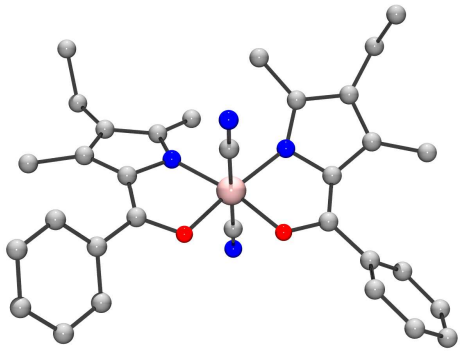

Figure SI2 Molecular structure of *CN trans CN* $\mathbf{2}^{\mathbf{CN}}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI2 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *CN trans CN* $\mathbf{2}^{\mathbf{CN}}$ (71 atoms), E = -1897.73539957 Hartree.

C	-5.47005	3.948	-0.74794
C	-5.51592	2.77784	-1.49595
C	-4.45495	4.14179	0.18368
C	-4.56189	1.79013	-1.29923
C	-3.48756	3.16808	0.36962
C	-3.55015	1.97492	-0.35576
C	-2.50163	0.97123	-0.16375
C	-2.66316	-0.41462	-0.12417
N	-1.45142	-1.07227	0.09646
C	-3.72977	-1.31369	0.14161
C	-1.7295	-2.29385	0.55719
C	-3.13363	-2.49691	0.56013
O	-1.30304	1.41299	0.02834
C	-5.19727	-1.06135	0.06838
C	-3.82054	-3.74211	1.03118
C	-4.16205	-3.7242	2.52373
C	-0.71824	-3.23067	1.11417
Si	-0.00114	0.14302	-0.07666
C	5.24545	4.14155	1.05983
C	4.21674	4.38827	0.15605
C	5.36236	2.89356	1.65974
C	3.30714	3.38971	-0.15039
C	4.46678	1.88326	1.34104
C	3.44203	2.12278	0.42413
C	2.45086	1.09202	0.10972
C	2.68844	-0.26853	-0.09317
N	1.51334	-0.96339	-0.38499
C	3.80182	-1.06987	-0.46061
C	1.85504	-2.10893	-0.97889
C	3.2684	-2.23032	-1.00964
O	1.22856	1.48581	-0.02865
C	5.25166	-0.73681	-0.37099
C	4.01304	-3.39929	-1.57368
C	4.33864	-4.47181	-0.53128
C	0.89376	-3.02641	-1.64624
H	-6.21903	4.71624	-0.89952
H	-6.2892	2.63869	-2.24158
H	-4.41387	5.05856	0.75914
H	-4.5708	0.89236	-1.9038

H	-2.68053	3.31153	1.07659
H	-5.45777	-0.07323	0.44985
H	-5.5632	-1.11794	-0.96086
H	-5.74307	-1.8042	0.65005
H	-4.73439	-3.89538	0.45014
H	-3.18627	-4.60746	0.81693
H	-4.83359	-2.897	2.76323
H	-4.64924	-4.65436	2.82553
H	-3.26516	-3.59985	3.13376
H	0.29348	-2.84733	1.01665
H	-0.91005	-3.36429	2.18218
H	-0.78085	-4.21514	0.64441
H	5.94929	4.92767	1.30629
H	4.12002	5.36444	-0.30328
H	6.14552	2.70967	2.3851
H	2.49026	3.57091	-0.83704
H	4.53036	0.92023	1.83112
H	5.44219	0.31255	-0.59792
H	5.64666	-0.92945	0.63076
H	5.82735	-1.34642	-1.0684
H	3.42665	-3.84552	-2.3821
H	4.9412	-3.05356	-2.0379
H	4.95913	-4.06341	0.26925
H	3.42835	-4.86357	-0.07162
H	4.87578	-5.30918	-0.98293
H	-0.13386	-2.69132	-1.53637
H	1.11413	-3.04651	-2.71732
H	0.98391	-4.04904	-1.27344
C	0.202	0.01865	1.83271
C	-0.20335	0.23175	-1.98803
N	0.30078	-0.11201	2.97678
N	-0.29964	0.23248	-3.13974

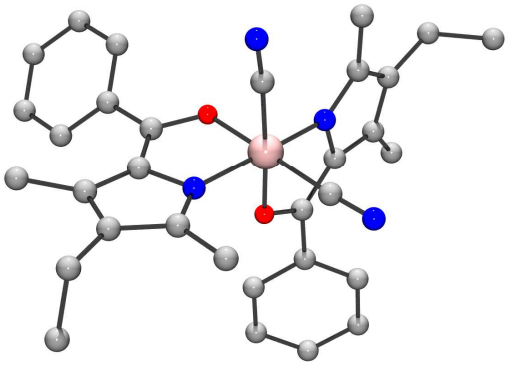

Figure SI3 Molecular structure of *N trans N* $\mathbf{2}^{\mathbf{CN}}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI3 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *N trans N* $\mathbf{2}^{\mathbf{CN}}$ (71 atoms), E = -1897.75191382 Hartree.

Si	0.04007	-0.13213	-1.23978
C	2.6113	4.3187	3.12709
C	1.37155	3.69292	3.20903
C	3.53875	3.90245	2.18003
C	1.06051	2.65195	2.34956
C	3.23921	2.8476	1.33007
C	2.00328	2.20578	1.41935
C	1.63742	1.12324	0.49909
C	2.44666	0.08232	0.05316
N	1.81036	-0.70976	-0.90015
C	3.72944	-0.45433	0.32613
C	2.65451	-1.68386	-1.25098
C	3.85776	-1.5616	-0.50427
O	0.43099	1.13878	0.04143
C	4.73375	-0.00088	1.33199
C	5.04811	-2.46136	-0.62245
C	6.03188	-2.02197	-1.7097
C	2.36642	-2.7193	-2.27699
C	-2.81336	-3.53111	3.84482
C	-1.98628	-4.03521	2.84636
C	-3.28653	-2.22726	3.76309
C	-1.63382	-3.23999	1.76811
C	-2.95141	-1.43313	2.67582
C	-2.13311	-1.93862	1.66449
C	-1.71773	-1.11079	0.52627
C	-2.49346	-0.20668	-0.19306
N	-1.75581	0.46168	-1.16802
C	-3.8572	0.16588	-0.30169
C	-2.59641	1.24155	-1.85332
C	-3.91399	1.08525	-1.34217
O	-0.49279	-1.23947	0.13986
C	-5.02551	-0.35337	0.46681
C	-5.12993	1.79717	-1.84713
C	-5.35055	3.16312	-1.19272
C	-2.19902	2.10882	-2.99184
H	2.84865	5.13979	3.79304
H	0.64353	4.02457	3.93943

H	4.49321	4.40747	2.09466
H	0.09241	2.16955	2.38873
H	3.94448	2.54495	0.56729
H	5.29033	-0.85573	1.72018
H	5.46652	0.68555	0.89692
H	4.26665	0.50835	2.17425
H	5.5681	-2.50112	0.33908
H	4.71948	-3.48545	-0.82111
H	6.41078	-1.01722	-1.51081
H	6.8856	-2.70159	-1.76589
H	5.55057	-2.00129	-2.68982
H	1.4905	-3.31426	-2.01592
H	2.15584	-2.26463	-3.24639
H	3.22049	-3.38562	-2.38763
H	-3.08076	-4.15206	4.69155
H	-1.61119	-5.04925	2.91268
H	-3.91148	-1.82512	4.55126
H	-0.97971	-3.61393	0.99123
H	-3.29505	-0.40821	2.62419
H	-5.23664	0.25389	1.35242
H	-5.92316	-0.33509	-0.15318
H	-4.86848	-1.37837	0.8011
H	-5.06124	1.91926	-2.93166
H	-6.01042	1.17116	-1.67784
H	-4.50269	3.82772	-1.37313
H	-6.24795	3.64654	-1.58608
H	-5.46562	3.06409	-0.11103
H	-1.41567	2.81101	-2.70545
H	-1.80182	1.51697	-3.81871
H	-3.05795	2.6725	-3.35233
C	0.66144	1.06392	-2.5894
C	-0.4368	-1.48336	-2.49941
N	1.12617	1.75294	-3.39175
N	-0.81574	-2.26858	-3.25742

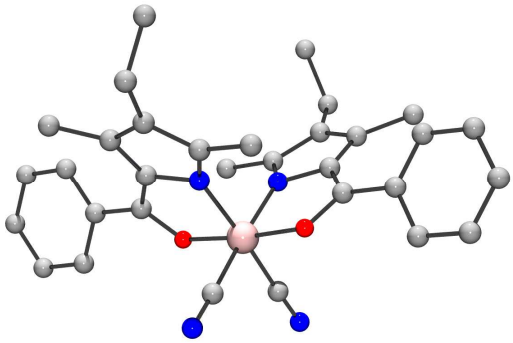

Figure SI4 Molecular structure of *O trans O* $\mathbf{2}^{\mathbf{CN}}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI4 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *O trans O* $\mathbf{2}^{\mathbf{CN}}$ (71 atoms), E = -1897,74762400 Hartree.

Si	-0.00006	-0.00005	-1.39153
C	-6.52537	1.29847	-0.54457
C	-5.78348	1.25141	-1.72037
C	-5.95659	0.88671	0.65482
C	-4.4762	0.79377	-1.70053
C	-4.65443	0.40919	0.67775
C	-3.9095	0.34871	-0.50185
C	-2.51535	-0.10165	-0.51436
C	-1.94099	-1.14044	0.20629
N	-0.57217	-1.248	-0.03276
C	-2.36595	-2.23326	1.01068
C	-0.13894	-2.34335	0.58815
C	-1.22329	-2.97968	1.25955
O	-1.71886	0.54779	-1.30676
C	-3.74947	-2.5815	1.44576
C	-1.1207	-4.23062	2.07414
C	-0.67615	-3.98183	3.51755
C	1.26479	-2.82915	0.54194
C	6.52531	-1.29856	-0.54502
C	5.95662	-0.8867	0.65438
C	5.78332	-1.25157	-1.72076
C	4.65447	-0.40916	0.67738
C	4.47604	-0.79392	-1.70086
C	3.90944	-0.34876	-0.50217
C	2.5153	0.10161	-0.51459
C	1.94101	1.14047	0.20601
N	0.57217	1.24801	-0.03292
C	2.36605	2.23335	1.01027
C	0.139	2.34342	0.58793
C	1.22341	2.9798	1.25919
O	1.71873	-0.5479	-1.30686
C	3.7496	2.58162	1.44521
C	1.1209	4.2308	2.07368
C	-1.26473	2.82922	0.54179
H	-7.54453	1.66587	-0.56182
H	-6.22391	1.57859	-2.65419
H	-6.52526	0.94474	1.57497

H	-3.88202	0.76544	-2.60477
H	-4.20012	0.11472	1.61481
H	-3.84589	-3.66067	1.57205
H	-4.00652	-2.12278	2.40552
H	-4.4948	-2.26102	0.71824
H	-2.08822	-4.73917	2.07905
H	-0.42634	-4.92673	1.59448
H	-1.37866	-3.32433	4.03439
H	-0.61434	-4.91853	4.07648
H	0.30606	-3.50473	3.55117
H	1.6358	-2.85523	-0.4823
H	1.92793	-2.17449	1.1139
H	1.33461	-3.82775	0.97037
H	7.54446	-1.66596	-0.56233
H	6.52536	-0.94467	1.57449
H	6.22367	-1.57883	-2.6546
H	4.20024	-0.11462	1.61446
H	3.88179	-0.76566	-2.60505
H	4.49487	2.2611	0.71763
H	3.84603	3.6608	1.57142
H	4.00675	2.12297	2.40497
H	-1.63584	2.8552	-0.48242
H	-1.92782	2.17461	1.11387
H	-1.33451	3.82786	0.97014
H	0.42648	4.92686	1.59404
C	0.6765	3.98213	3.51716
H	0.61475	4.91888	4.07601
H	-0.30571	3.50504	3.55092
H	1.37906	3.32468	4.03398
H	2.08841	4.73936	2.07845
C	0.37849	1.33344	-2.70245
C	-0.37873	-1.33365	-2.7023
N	0.6314	2.15551	-3.47347
N	-0.63171	-2.15578	-3.47324

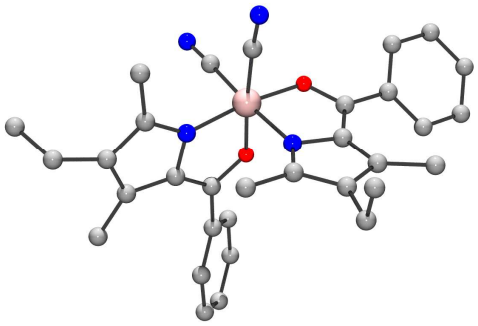

Figure SI5 Molecular structure of *all cis* $\mathbf{2}^{CN}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI5 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *all cis* $\mathbf{2}^{CN}$ (71 atoms), E = - 1897.74915723 Hartree.

Si	0.03186	-0.52995	-1.1913
C	1.90461	5.24995	1.75788
C	2.43614	4.14097	2.40495
C	1.22672	5.09551	0.55288
C	2.30916	2.88037	1.83962
C	1.07989	3.83655	-0.00608
C	1.64022	2.72215	0.62509
C	1.43899	1.39977	0.02309
C	2.35504	0.34587	-0.0365
N	1.81537	-0.78638	-0.64656
C	3.74068	0.14646	0.17059
C	2.81066	-1.66516	-0.83101
C	4.01699	-1.12818	-0.3169
O	0.30065	1.18633	-0.53035
C	4.74959	1.0992	0.72
C	5.35792	-1.79428	-0.37045
C	6.07933	-1.59573	-1.70571
C	2.65844	-2.9756	-1.51355
C	-6.33021	1.57484	-1.60197
C	-5.60617	0.85131	-2.54415
C	-5.8089	1.77953	-0.33011
C	-4.36513	0.33044	-2.21713
C	-4.57507	1.2441	0.00914
C	-3.85206	0.50425	-0.92806
C	-2.52315	-0.03072	-0.62249
C	-2.08422	-0.59781	0.57337
N	-0.73547	-0.93868	0.52581
C	-2.64501	-1.06856	1.78689
C	-0.4408	-1.58513	1.65633
C	-1.6001	-1.67815	2.47147
O	-1.65772	0.01178	-1.5781
C	-4.06324	-1.01058	2.24806
C	-1.6826	-2.3698	3.79746
H	-2.49387	-1.92955	4.3833
C	0.89743	-2.15026	1.97638
H	2.01024	6.23471	2.19733
H	2.94364	4.25671	3.35491
H	0.80698	5.95897	0.05141

H	2.69665	2.01121	2.35513
H	0.5429	3.69805	-0.93563
H	4.83	1.02666	1.80906
H	5.73659	0.88399	0.30943
H	4.50347	2.13313	0.47878
H	5.98238	-1.41361	0.44228
H	5.24349	-2.86451	-0.17393
H	7.05227	-2.09269	-1.70396
H	5.49394	-2.00017	-2.53394
H	6.23938	-0.53498	-1.91031
H	3.60318	-3.51688	-1.49939
H	1.8903	-3.5966	-1.05218
H	2.35715	-2.83521	-2.55426
H	-7.29629	1.98981	-1.86382
H	-6.00717	0.70058	-3.53894
H	-6.35947	2.36579	0.39557
H	-3.78136	-0.21803	-2.94498
H	-4.15027	1.43156	0.9865
H	-4.28516	-1.85721	2.89888
H	-4.26906	-0.10077	2.82064
H	-4.76291	-1.03652	1.41301
H	-0.77079	-2.17561	4.37087
H	1.13405	-2.98493	1.3118
H	1.68988	-1.40887	1.86761
H	0.91283	-2.52466	2.99923
C	-1.89901	-3.88061	3.68122
H	-1.95722	-4.34762	4.66733
H	-2.82402	-4.10212	3.14466
H	-1.08415	-4.35462	3.12983
C	-0.34616	-2.31677	-1.7396
C	0.59178	0.0364	-2.92135
N	0.98866	0.35991	-3.95663
N	-0.6468	-3.39246	-2.03501

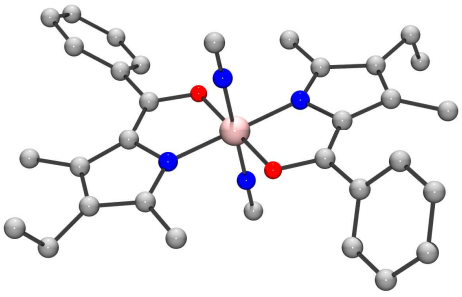

Figure SI6 Molecular structure of *all trans* $\mathbf{2}^{NC}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI6 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *all trans* $\mathbf{2}^{NC}$ (71 atoms), E = -1897.74095818 Hartree.

C	-5.88266	3.19321	0.35923
C	-4.8336	3.49286	-0.50364
C	-5.85014	2.02846	1.11597
C	-3.75262	2.63227	-0.60834
C	-4.78002	1.15259	0.99938
C	-3.72896	1.44663	0.13025
C	-2.5632	0.56227	0.02265
O	-1.39888	1.13144	0.0454
C	-2.56898	-0.8191	-0.11249
N	-1.28392	-1.35285	-0.13822
C	-3.51017	-1.86221	-0.31884
C	-1.38666	-2.66574	-0.32531
C	-2.76055	-3.02373	-0.44484
C	-4.99287	-1.75672	-0.43643
C	-3.27961	-4.41115	-0.65668
C	-3.54789	-5.16476	0.64841
C	-0.22088	-3.58168	-0.41957
C	5.89505	-3.21473	0.20189
C	4.90505	-3.37766	-0.76168
C	5.80288	-2.18173	1.12639
C	3.82319	-2.51252	-0.79998
C	4.73271	-1.29965	1.07926
C	3.74098	-1.45618	0.11059
C	2.57627	-0.56501	0.07265
O	1.4158	-1.12804	-0.05694
Si	0.00779	0.00084	-0.00199
C	2.58215	0.82045	0.15286
N	1.29727	1.35556	0.14181
C	3.52679	1.88085	0.16511
C	1.40244	2.68096	0.17007
C	2.77887	3.04894	0.18826
C	5.01553	1.79511	0.1192
C	3.30059	4.45228	0.18379
C	0.23944	3.60471	0.16781
H	-6.72184	3.87284	0.44776
H	-4.85713	4.40209	-1.092
H	-6.65554	1.80459	1.80484
H	-2.92744	2.85731	-1.27181
H	-4.73572	0.25814	1.60754
H	-5.37829	-2.5392	-1.09225

H	-5.48706	-1.87732	0.53227
H	-5.29955	-0.79315	-0.84247
H	-4.20248	-4.36499	-1.24202
H	-2.57252	-4.9789	-1.26793
H	-3.92792	-6.16991	0.45082
H	-2.6373	-5.25827	1.24441
H	-4.28434	-4.63789	1.25887
H	0.31927	-3.41543	-1.35501
H	0.48263	-3.4039	0.39245
H	-0.5475	-4.62006	-0.39009
H	6.73432	-3.89911	0.23665
H	4.97499	-4.18438	-1.48121
H	6.56133	-2.06686	1.89118
H	3.04287	-2.63243	-1.54064
H	4.64125	-0.51054	1.81474
H	5.43273	2.67483	-0.37236
H	5.44946	1.74737	1.12267
H	5.35328	0.91289	-0.42412
H	2.6967	5.06855	0.85729
H	-0.2427	3.60781	-0.813
H	-0.51044	3.29199	0.89281
H	0.55987	4.62068	0.39535
N	0.05614	0.14432	-1.82877
N	-0.04024	-0.14284	1.82211
C	0.08938	0.2395	-2.99535
C	-0.07295	-0.23613	2.9888
H	4.30923	4.46238	0.60481
C	3.32114	5.08954	-1.20768
H	3.70864	6.1103	-1.16675
H	3.94892	4.51439	-1.89161
H	2.3189	5.12622	-1.64

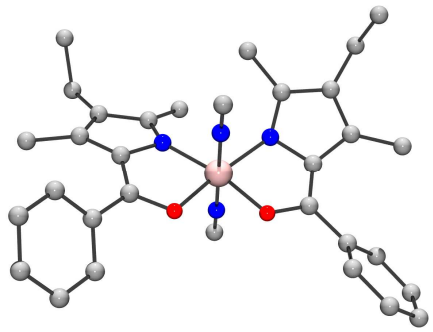

Figure SI7 Molecular structure of *CN trans CN* **2**^{NC} (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI7 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *NC trans NC* **2**^{NC} (71 atoms), E = -1897.72358653 Hartree.

C	-5.44661	3.95254	-0.75132
C	-5.50348	2.77918	-1.4935
C	-4.42401	4.14555	0.17229
C	-4.55276	1.78785	-1.29894
C	-3.46012	3.16799	0.35603
C	-3.53343	1.97182	-0.36349
C	-2.48868	0.96407	-0.17514
C	-2.65388	-0.42181	-0.13783
N	-1.44293	-1.07701	0.08213
C	-3.72005	-1.31844	0.13707
C	-1.71874	-2.29499	0.55327
C	-3.12261	-2.49906	0.56109
O	-1.28989	1.40047	0.01913
C	-5.18775	-1.06723	0.06464
C	-3.80721	-3.74262	1.03994
C	-4.15578	-3.71346	2.5307
C	-0.70814	-3.23205	1.1108
Si	-0.0006	0.13205	-0.07832
C	5.21642	4.15435	1.05412
C	4.18132	4.39443	0.1558
C	5.34483	2.90698	1.65292
C	3.27686	3.38993	-0.14626
C	4.45422	1.89089	1.33862
C	3.42303	2.12369	0.42718
C	2.43738	1.08659	0.11806
C	2.68033	-0.27435	-0.07844
N	1.50704	-0.9683	-0.37014
C	3.79426	-1.07261	-0.45033
C	1.84786	-2.11028	-0.97088
C	3.26125	-2.23174	-1.00275
O	1.21493	1.47357	-0.02605
C	5.24383	-0.73883	-0.35976
C	4.00606	-3.39968	-1.56871
C	4.32902	-4.47566	-0.52903
C	0.88867	-3.02671	-1.64218
H	-6.19287	4.72376	-0.90119
H	-6.28276	2.64031	-2.23292
H	-4.37444	5.06478	0.74314
H	-4.57044	0.88741	-1.8993
H	-2.64728	3.31043	1.05649
H	-5.44875	-0.07862	0.44472

H	-5.5545	-1.1257	-0.96423
H	-5.73262	-1.80956	0.64783
H	-4.71798	-3.90457	0.45627
H	-3.16885	-4.60743	0.83597
H	-4.83129	-2.88664	2.76017
H	-4.64114	-4.64273	2.83828
H	-3.2622	-3.58066	3.14388
H	0.30025	-2.83472	1.04095
H	-0.92072	-3.3925	2.17107
H	-0.75069	-4.20715	0.61944
H	5.91628	4.94507	1.29716
H	4.07571	5.37011	-0.30264
H	6.13311	2.72807	2.37396
H	2.45504	3.56553	-0.82844
H	4.52704	0.92821	1.82808
H	5.43376	0.31086	-0.586
H	5.63847	-0.93169	0.64212
H	5.82041	-1.3476	-1.05716
H	3.42114	-3.84335	-2.37963
H	4.93542	-3.05343	-2.03017
H	4.94823	-4.06998	0.27389
H	3.41757	-4.86814	-0.07225
H	4.86649	-5.31217	-0.98199
H	-0.13791	-2.68585	-1.5435
H	1.11998	-3.05433	-2.71081
H	0.97176	-4.04791	-1.26379
N	-0.18603	0.21649	-1.89867
N	0.18564	0.01879	1.74059
C	-0.28289	0.25279	-3.06494
C	0.28339	-0.07589	2.90349

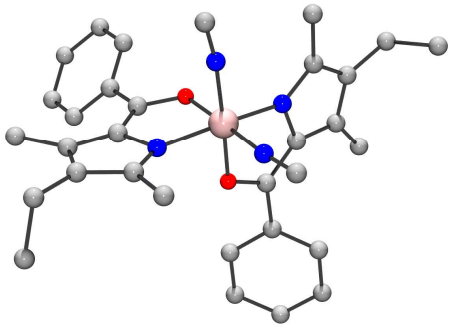

Figure SI8 Molecular structure of *N trans N* **2**^{NC} (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI8 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *N trans N* **2**^{NC} (71 atoms), E = -1897.74094720 Hartree.

Si	0.03878	-0.14382	-1.25989
C	2.52634	4.33617	3.11822
C	1.29235	3.69736	3.18515
C	3.46779	3.93225	2.17969
C	1.00124	2.65576	2.3195
C	3.18804	2.87696	1.3235
C	1.95812	2.22187	1.39795
C	1.61246	1.13739	0.47201
C	2.43496	0.10494	0.03095
N	1.81079	-0.69214	-0.92462
C	3.72442	-0.41504	0.30547
C	2.66902	-1.65256	-1.27863
C	3.86921	-1.51726	-0.52814
O	0.41047	1.14043	0.00481
C	4.72065	0.04837	1.31478
C	5.07247	-2.39996	-0.64606
C	6.06394	-1.93184	-1.7142
C	2.40506	-2.68933	-2.30989
C	-2.72316	-3.49164	3.89897
C	-1.8943	-4.00066	2.90447
C	-3.21853	-2.19753	3.79612
C	-1.5622	-3.22011	1.80917
C	-2.9035	-1.41847	2.6921
C	-2.08346	-1.9292	1.68479
C	-1.68868	-1.1166	0.52854
C	-2.48034	-0.23364	-0.19957
N	-1.75712	0.42517	-1.19019
C	-3.84983	0.11808	-0.30675
C	-2.61167	1.17971	-1.88627
C	-3.92471	1.01608	-1.36412
O	-0.4667	-1.23721	0.13285
C	-5.00631	-0.40166	0.47916
C	-5.15292	1.70283	-1.87435
C	-5.37733	3.08486	-1.256
C	-2.23843	2.03356	-3.04291
H	2.7483	5.15758	3.78905
H	0.55324	4.01926	3.90875
H	4.41793	4.44717	2.10589
H	0.03787	2.16323	2.34702
H	3.90465	2.58402	0.56757

H	5.28766	-0.80054	1.70104
H	5.44544	0.74573	0.88372
H	4.24515	0.54848	2.15784
H	5.58149	-2.44747	0.32111
H	4.75973	-3.4251	-0.86352
H	6.42709	-0.92532	-1.49573
H	6.92728	-2.59931	-1.76958
H	5.59481	-1.90271	-2.70004
H	1.57686	-3.33899	-2.02396
H	2.13143	-2.2344	-3.26219
H	3.29277	-3.30185	-2.45931
H	-2.97463	-4.1009	4.75898
H	-1.50192	-5.00692	2.98724
H	-3.84499	-1.79109	4.58089
H	-0.90684	-3.59716	1.03485
H	-3.26431	-0.40045	2.62382
H	-5.22147	0.2213	1.35285
H	-5.9076	-0.40957	-0.13576
H	-4.83272	-1.41695	0.83434
H	-5.09904	1.79487	-2.96277
H	-6.02575	1.07461	-1.67625
H	-4.5377	3.75116	-1.46617
H	-6.28396	3.54957	-1.65086
H	-5.47734	3.01517	-0.17054
H	-1.49151	2.77671	-2.76293
H	-1.80343	1.43847	-3.84706
H	-3.11718	2.54926	-3.42665
N	0.57582	0.99257	-2.55676
N	-0.37172	-1.45494	-2.43418
C	1.07569	1.68627	-3.35692
C	-0.7895	-2.25777	-3.17744

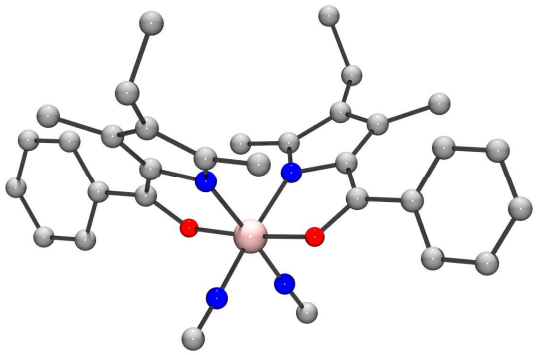

Figure SI9 Molecular structure of *O trans O* **2**^{NC} (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI9 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *O trans O* **2**^{NC} (71 atoms), E = -1897.73717409 Hartree.

Si	-0.00007	-0.00005	-1.41028
C	-6.52652	1.23693	-0.52598
C	-5.79115	1.19696	-1.70612
C	-5.9464	0.83127	0.67006
C	-4.4793	0.75217	-1.69403
C	-4.63943	0.3667	0.68521
C	-3.90102	0.31284	-0.49877
C	-2.50299	-0.12509	-0.52019
C	-1.91374	-1.15597	0.19992
N	-0.54881	-1.25304	-0.05667
C	-2.32114	-2.25338	1.00736
C	-0.09978	-2.34825	0.5526
C	-1.1705	-2.99292	1.23853
O	-1.71925	0.52694	-1.32129
C	-3.69595	-2.61011	1.46264
C	-1.04784	-4.24488	2.04869
C	-0.57337	-3.99739	3.48274
C	1.30402	-2.83071	0.48204
C	6.52645	-1.23701	-0.52643
C	5.94643	-0.83125	0.66963
C	5.79099	-1.19713	-1.70652
C	4.63947	-0.36667	0.68485
C	4.47914	-0.75232	-1.69435
C	3.90097	-0.3129	-0.49908
C	2.50294	0.12504	-0.52042
C	1.91376	1.15599	0.19965
N	0.5488	1.25306	-0.05683
C	2.32124	2.25347	1.00697
C	0.09984	2.34832	0.55238
C	1.17062	2.99303	1.23817
O	1.71912	-0.52704	-1.3214
C	3.69609	2.61022	1.4621
C	1.04804	4.24507	2.04824
C	-1.30396	2.83079	0.48191
H	-7.54937	1.59416	-0.53722
H	-6.24039	1.51969	-2.63732
H	-6.50999	0.88404	1.59364

H	-3.88982	0.72945	-2.60152
H	-4.17648	0.07752	1.61968
H	-3.78188	-3.68907	1.59765
H	-3.94445	-2.14683	2.42248
H	-4.45338	-2.30066	0.74274
H	-2.01375	-4.75591	2.07342
H	-0.36206	-4.93876	1.55354
H	-1.26635	-3.34242	4.01542
H	-0.49732	-4.93481	4.03877
H	0.40815	-3.51788	3.4963
H	1.66434	-2.83293	-0.54595
H	1.97248	-2.18906	1.06253
H	1.37844	-3.83851	0.88779
H	7.5493	-1.59426	-0.53773
H	6.5101	-0.88396	1.59317
H	6.24015	-1.51994	-2.63772
H	4.1766	-0.07741	1.61932
H	3.88959	-0.72967	-2.6018
H	4.45345	2.3007	0.74216
H	3.78204	3.68919	1.59702
H	3.94466	2.14701	2.42195
H	-1.66437	2.83293	-0.54606
H	-1.97238	2.18919	1.0625
H	-1.37834	3.83863	0.88758
H	0.36221	4.9389	1.55309
C	0.57371	3.99771	3.48236
H	0.49772	4.93517	4.03831
H	-0.4078	3.5182	3.49605
H	1.26675	3.34278	4.01502
H	2.01396	4.75609	2.07283
C	0.57438	2.09563	-3.44133
C	-0.5747	-2.09591	-3.4411
N	0.33659	1.26141	-2.65494
N	-0.33683	-1.26162	-2.6548

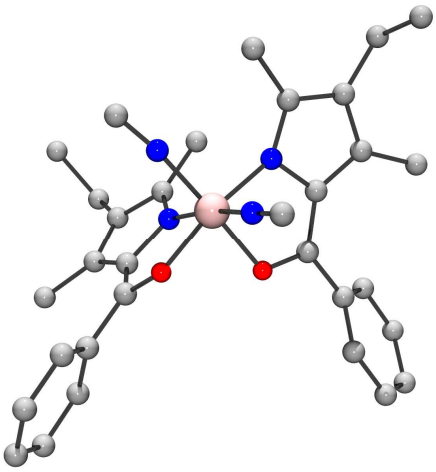

Figure SI10 Molecular structure of *all cis* $\mathbf{2}^{\mathbf{NC}}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI10 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *all cis* $\mathbf{2}^{\mathbf{NC}}$ (71 atoms), E = -1897.73830661 Hartree.

Si	0.03179	-0.52841	-1.2075
C	1.8575	5.241	1.77505
C	2.39684	4.13216	2.4159
C	1.18127	5.08862	0.56887
C	2.2793	2.87396	1.84322
C	1.04412	3.83191	0.00245
C	1.6123	2.71793	0.62736
C	1.42212	1.39841	0.01596
C	2.34378	0.34953	-0.04741
N	1.81086	-0.777	-0.67091
C	3.73027	0.15558	0.15934
C	2.8108	-1.6471	-0.86819
C	4.01397	-1.11069	-0.34485
O	0.28885	1.18187	-0.54506
C	4.73277	1.10599	0.72425
C	5.3591	-1.7682	-0.40426
C	6.09089	-1.5328	-1.72792
C	2.67046	-2.95086	-1.56617
C	-6.33606	1.53956	-1.5797
C	-5.60991	0.82831	-2.52958
C	-5.81183	1.73887	-0.30819
C	-4.36399	0.31415	-2.21051
C	-4.57289	1.21012	0.02289
C	-3.84772	0.48228	-0.92198
C	-2.51425	-0.04595	-0.62443
C	-2.0665	-0.61444	0.56775
N	-0.7178	-0.94693	0.50876
C	-2.61723	-1.0966	1.78161
C	-0.41135	-1.60055	1.63152
C	-1.56447	-1.70512	2.45476
O	-1.65458	0.00464	-1.58328
C	-4.03231	-1.04728	2.25324
C	-1.63407	-2.40693	3.7762
H	-2.44371	-1.9754	4.37076
C	0.9312	-2.16207	1.94021
H	1.95574	6.22393	2.22029
H	2.90301	4.24609	3.3668
H	0.75529	5.95189	0.07233
H	2.67273	2.00467	2.35395
H	0.50857	3.69449	-0.9281

H	4.80828	1.02113	1.81281
H	5.72265	0.89973	0.31609
H	4.4834	2.14174	0.49418
H	5.97495	-1.40425	0.42264
H	5.24941	-2.84346	-0.23485
H	7.06647	-2.02461	-1.73013
H	5.51485	-1.91937	-2.57118
H	6.24725	-0.46646	-1.90471
H	3.6365	-3.45003	-1.62181
H	1.96406	-3.61248	-1.06325
H	2.29275	-2.80746	-2.57981
H	-7.30607	1.94927	-1.83524
H	-6.01323	0.68201	-3.52412
H	-6.36414	2.31581	0.42361
H	-3.77828	-0.22447	-2.94415
H	-4.14599	1.39382	1.00003
H	-4.2452	-1.89665	2.9035
H	-4.2389	-0.13996	2.82953
H	-4.73779	-1.07469	1.42305
H	-0.71957	-2.21189	4.34504
H	1.17419	-2.98146	1.25955
H	1.71822	-1.41278	1.84635
H	0.94926	-2.55566	2.95578
C	-1.84323	-3.91799	3.65075
H	-1.89167	-4.39257	4.6338
H	-2.771	-4.14056	3.11937
H	-1.0299	-4.38354	3.08992
N	0.5433	0.01122	-2.84826
N	-0.28854	-2.22562	-1.73226
C	0.91152	0.37429	-3.89864
C	-0.64006	-3.29823	-2.04478

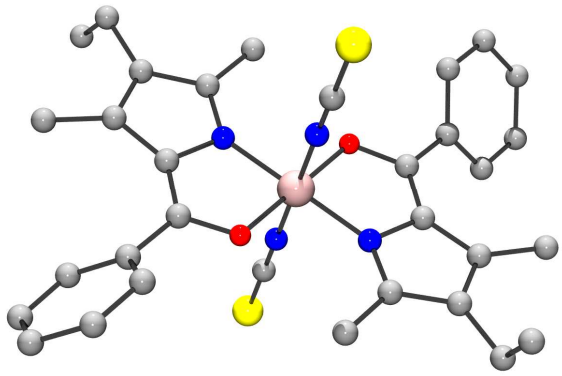

Figure SI11 Molecular structure of *all trans* **3**^{NCS} (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI11 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *all trans* **3**^{NCS} (71 atoms), E = -2694.27620040 Hartree.

C	5.87584	3.18684	-0.50867
C	4.81879	3.53745	0.32476
C	5.85428	1.97461	-1.18718
C	3.74119	2.68012	0.47803
C	4.78729	1.1031	-1.02143
C	3.72807	1.44794	-0.18082
C	2.56541	0.56746	-0.02505
O	1.39817	1.13101	-0.08168
C	2.5728	-0.80473	0.18511
N	1.28793	-1.34001	0.23319
C	3.51519	-1.83362	0.45122
C	1.39363	-2.64172	0.48965
C	2.76783	-2.98858	0.63488
C	4.99693	-1.71934	0.57139
C	3.28882	-4.36193	0.92118
C	3.57297	-5.17748	-0.34271
C	0.23211	-3.55781	0.62789
C	-5.88746	-3.23467	-0.11959
C	-4.90684	-3.35935	0.85917
C	-5.78682	-2.23813	-1.0824
C	-3.82626	-2.492	0.87513
C	-4.71794	-1.35386	-1.05879
C	-3.73578	-1.47096	-0.07445
C	-2.57425	-0.57591	-0.0612
O	-1.41303	-1.12774	0.11369
Si	-0.00598	0.0002	0.01362
C	-2.5807	0.8039	-0.21272
N	-1.29604	1.34161	-0.21648
C	-3.52641	1.86088	-0.29226
C	-1.40311	2.66407	-0.31927
C	-2.77988	3.02726	-0.37176
C	-5.01535	1.7769	-0.25265
C	-3.30384	4.42758	-0.44848
C	-0.24296	3.59095	-0.35683
H	6.71251	3.86336	-0.63584
H	4.83352	4.48347	0.85213

H	6.66546	1.71007	-1.85445
H	2.91042	2.94547	1.11915
H	4.75236	0.17128	-1.57126
H	5.37881	-2.46272	1.27307
H	5.49663	-1.89492	-0.38597
H	5.30032	-0.73389	0.92351
H	4.20516	-4.28348	1.51317
H	2.57698	-4.90101	1.55236
H	3.9512	-6.17133	-0.09211
H	2.66956	-5.30075	-0.94413
H	4.31627	-4.68002	-0.96923
H	-0.28413	-3.37974	1.57512
H	-0.49271	-3.39618	-0.16798
H	0.56088	-4.59576	0.60857
H	-6.72576	-3.92085	-0.13615
H	-4.98325	-4.1377	1.60861
H	-6.53722	-2.15414	-1.859
H	-3.05389	-2.58346	1.62804
H	-4.61983	-0.59498	-1.82456
H	-5.43502	2.67856	0.19502
H	-5.44264	1.68332	-1.25568
H	-5.35706	0.92107	0.32888
H	-2.69556	5.00706	-1.15006
H	0.22245	3.66157	0.62964
H	0.52104	3.23671	-1.04693
H	-0.56311	4.58856	-0.65482
N	-0.0726	0.23895	1.81622
N	0.05985	-0.23996	-1.78688
C	-0.13063	0.39948	2.98153
C	0.1077	-0.40074	-2.95242
S	-0.20884	0.61698	4.56285
S	0.17228	-0.61849	-4.53423
H	-4.30905	4.41261	-0.87727
C	-3.33585	5.13917	0.90625
H	-3.72456	6.15538	0.80713
H	-3.96781	4.60072	1.61573
H	-2.33694	5.20125	1.34328

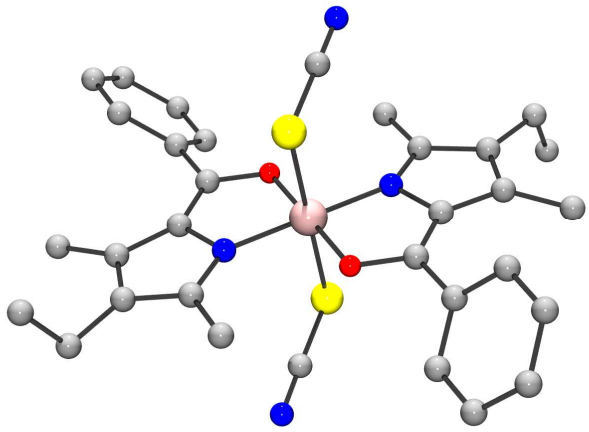

Figure SI12 Molecular structure of *all trans* $\mathbf{3}^{SCN}$ (H atoms omitted) at the MPW1PW91/6-311G(d,p) level.

Table SI12 Cartesian coordinates of the optimized (DFT MPW1PW91/6-311G(d,p)) molecular structure of *all trans* $\mathbf{3}^{SCN}$ (71 atoms), E = -2694.21886477 Hartree.

C	5.87169	-3.18379	-0.1023
C	4.77966	-3.42348	-0.92982
C	5.87489	-2.08197	0.74412
C	3.69228	-2.56521	-0.91178
C	4.7972	-1.20879	0.75241
C	3.70354	-1.44033	-0.08302
C	2.54	-0.55255	-0.06034
O	1.36488	-1.1245	-0.0356
C	2.535	0.82836	-0.06969
N	1.24722	1.3627	0.04909
C	3.4665	1.89345	-0.20244
C	1.3527	2.69346	0.04099
C	2.72032	3.05735	-0.12738
C	4.93526	1.8064	-0.44031
C	3.22462	4.46359	-0.20489
C	3.68852	5.01806	1.14449
C	0.22669	3.6493	0.18675
C	-5.85429	3.2192	0.31801
C	-4.80735	3.44285	-0.57035
C	-5.8323	2.1122	1.15783
C	-3.7367	2.56448	-0.62086
C	-4.77414	1.21698	1.09919
C	-3.72616	1.43493	0.20382
C	-2.5746	0.53445	0.14803
O	-1.40036	1.10426	0.10406
Si	-0.01453	-0.00824	0.06162
C	-2.56854	-0.84771	0.11145
N	-1.27402	-1.3733	0.06787
C	-3.50071	-1.91441	0.01498
C	-1.36887	-2.70156	-0.03366
C	-2.74363	-3.07309	-0.06002
C	-4.98877	-1.83532	-0.03137
C	-3.25703	-4.47416	-0.17875
C	-0.20918	-3.6219	-0.13763

H	6.71583	-3.86286	-0.11013
H	4.77463	-4.28509	-1.5862
H	6.71338	-1.90785	1.40726
H	2.83533	-2.74457	-1.54799
H	4.78012	-0.36782	1.43364
H	5.27345	2.66603	-1.02118
H	5.5	1.80837	0.49651
H	5.20428	0.90088	-0.98323
H	4.05273	4.50969	-0.91824
H	2.44266	5.10558	-0.61801
H	4.04166	6.04685	1.044
H	2.87709	5.00988	1.87568
H	4.50446	4.41929	1.55486
H	-0.06433	4.02186	-0.79937
H	-0.64173	3.18152	0.63968
H	0.53962	4.50008	0.79415
H	-6.68445	3.91415	0.36149
H	-4.82305	4.30714	-1.22296
H	-6.63577	1.95011	1.86597
H	-2.9132	2.73118	-1.30491
H	-4.7356	0.37027	1.7725
H	-5.39786	-2.67828	-0.58908
H	-5.42422	-1.86729	0.97202
H	-5.32982	-0.91594	-0.5069
H	-4.26333	-4.52231	0.24481
H	0.30423	-3.48498	-1.09238
H	0.50717	-3.43704	0.66077
H	-0.54635	-4.6551	-0.07461
C	-0.15043	1.57419	-2.69191
C	0.1036	-1.57154	2.81228
S	-0.1113	-0.0578	-2.3103
S	0.06367	0.05746	2.40831
N	-0.19735	2.69963	-2.97178
N	0.12931	-2.69066	3.11611
H	-2.64681	-5.13659	0.44211
C	-3.283	-4.99631	-1.61716
H	-3.91501	-4.36961	-2.25018
H	-2.28294	-4.99902	-2.0562
H	-3.66971	-6.01723	-1.65542

Crystal structure of **4**

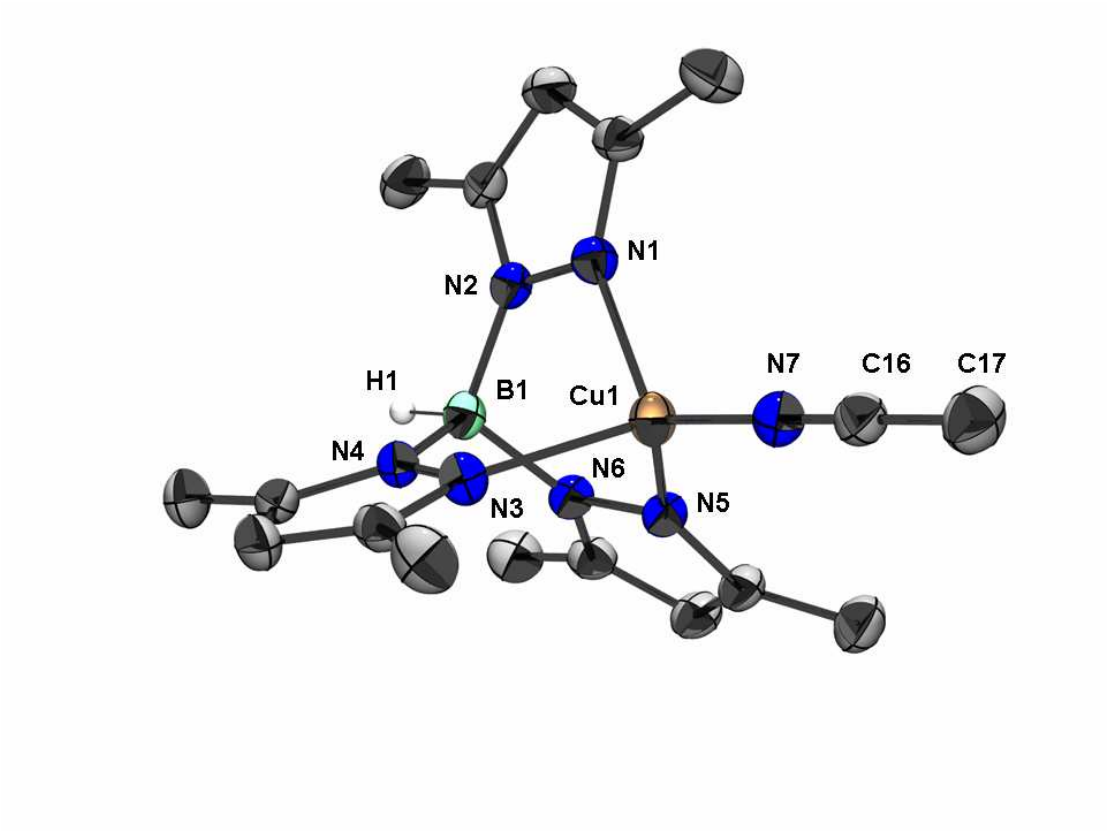

Figure SI13: Molecular structure of **4** in the crystal of **4·MeCN**; ellipsoids set at 50% probability level; C-bound H atoms and solvent molecule are omitted for clarity. Selected bond lengths [Å] bond angles and torsion angles [deg]: Cu1-N1 2.091(2), Cu1-N3 2.049(2), Cu1-N5 2.069(2), Cu1-N7 1.885(2), N1-N2 1.376(3), N3-N4 1.377(3), N5-N6 1.372(3), B1-N2 1.556(4), B1-N4 1.552(3), B1-N6 1.550(4), N7-C16 1.142(4); N1-Cu1-N3 91.4(1), N1-Cu-N5 90.5(1), N1-Cu1-N7 124.0(1), N3-Cu1-N5 89.7(1), N3-Cu1-N7 126.8(1), N5-Cu1-N7 123.9(1), N2-B1-N4 109.3(2), N2-B1-N6 109.2(2), N4-B1-N6 109.1(4), Cu1-N7-C16 179.7(3); B1-N2-N1-Cu1 1.7(3), B1-N4-N3-Cu1 0.9(3), B1-N6-N5-Cu1 2.3(3).

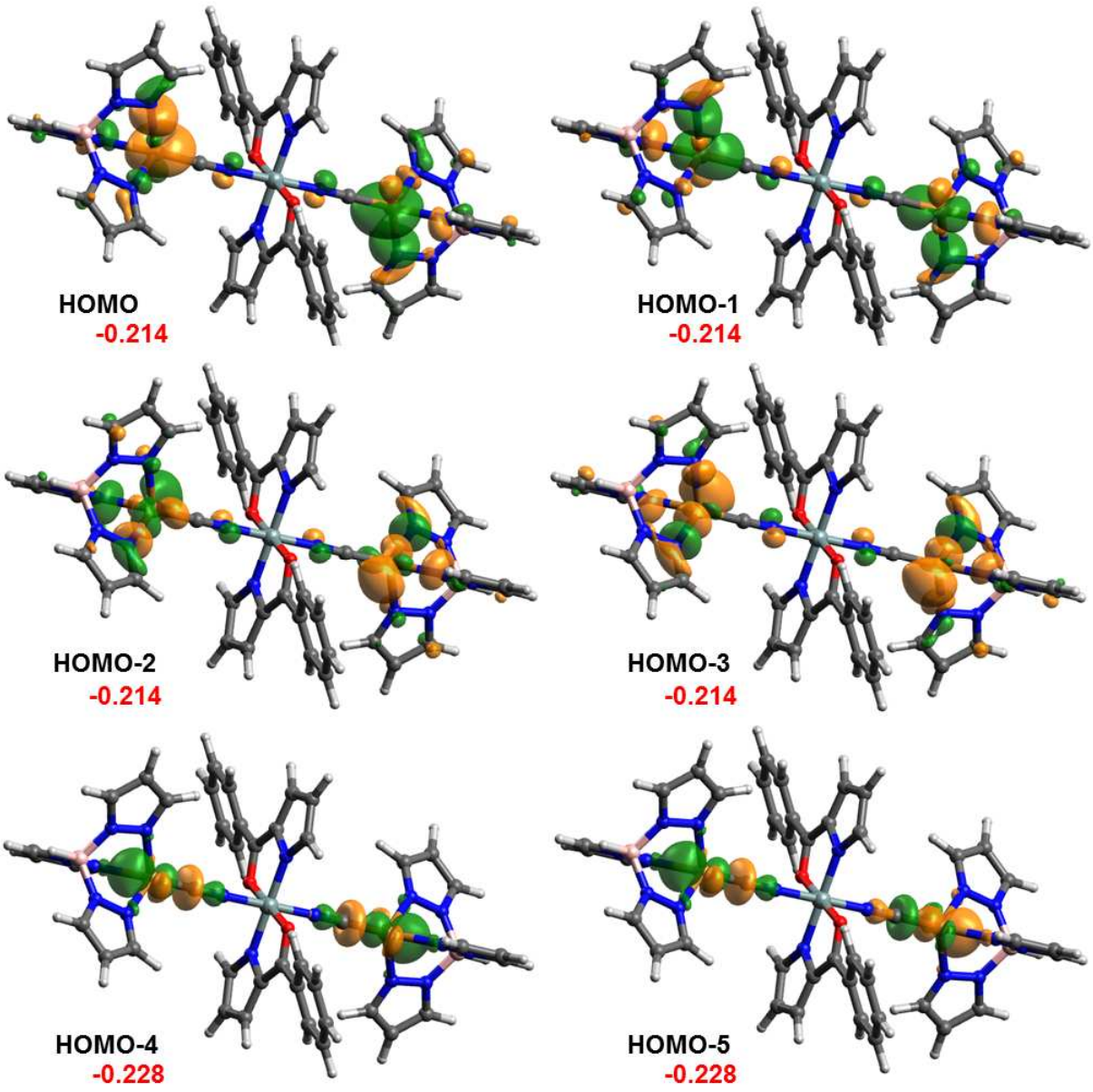

Figure SI14: Highest occupied MOs (HOMO – HOMO-5) of model compound **5'** (isosurface value: 0.03, energies in eV).

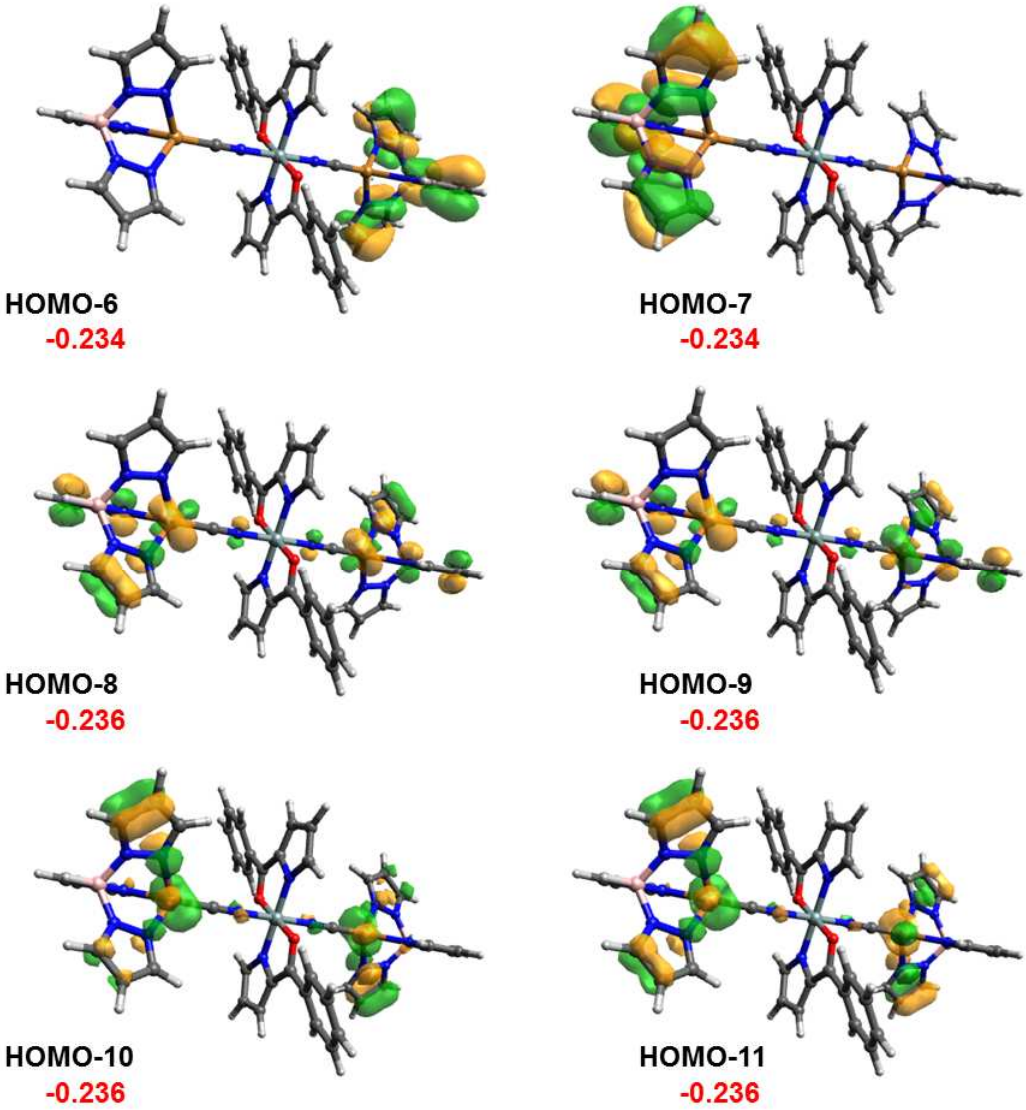

Figure SI15: Highest occupied MOs (continued, HOMO-6 – HOMO-11) of model compound **5'** (isosurface value: 0.03, energies in eV).

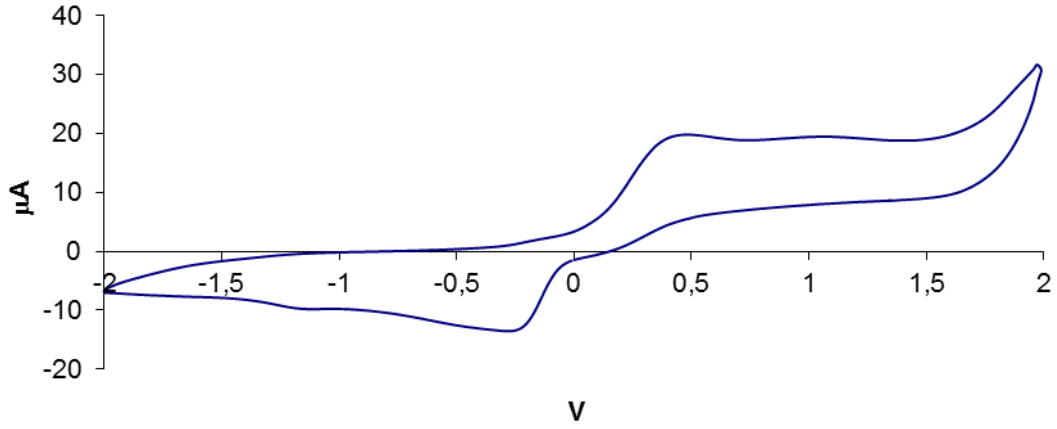

Figure SI16: CV trace of an acetonitrile solution of [Tp*Cu(NCMe)] (10^{-4} M) at a scan rate of 100 mV s^{-1} (supporting electrolyte: 0.1 M Bu_4NPF_6; Ar atmosphere) using a three electrode arrangement with Pt as working and counter electrode and a non-aqueous Ag/Ag^+-reference electrode. The potential was internally referred to the Fc/Fc^+ couple.

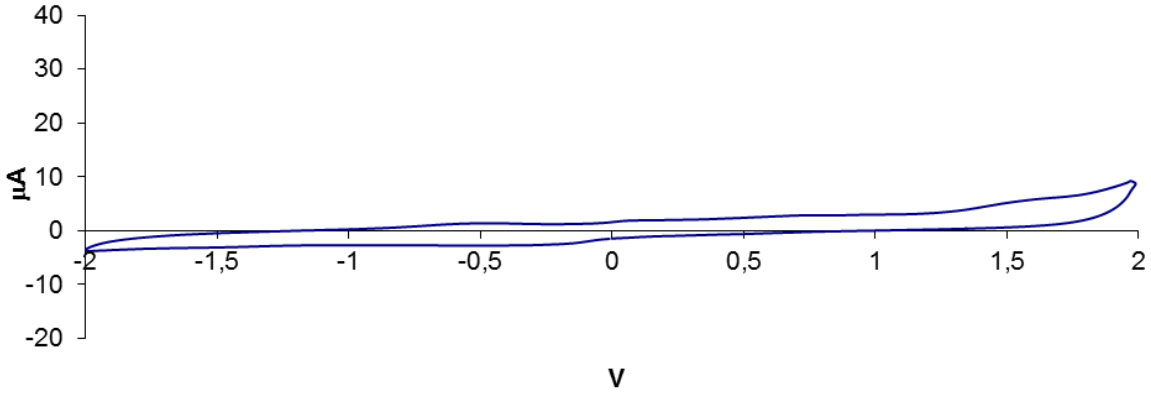

Figure SI17: CV trace of an acetonitrile solution of [Tp*$_2$Cu] (10^{-4} M) at a scan rate of 100 mV s^{-1} (supporting electrolyte: 0.1 M Bu_4NPF_6; Ar atmosphere) using a three electrode arrangement with Pt as working and counter electrode and a non-aqueous Ag/Ag^+-reference electrode. The potential was internally referred to the Fc/Fc^+ couple.

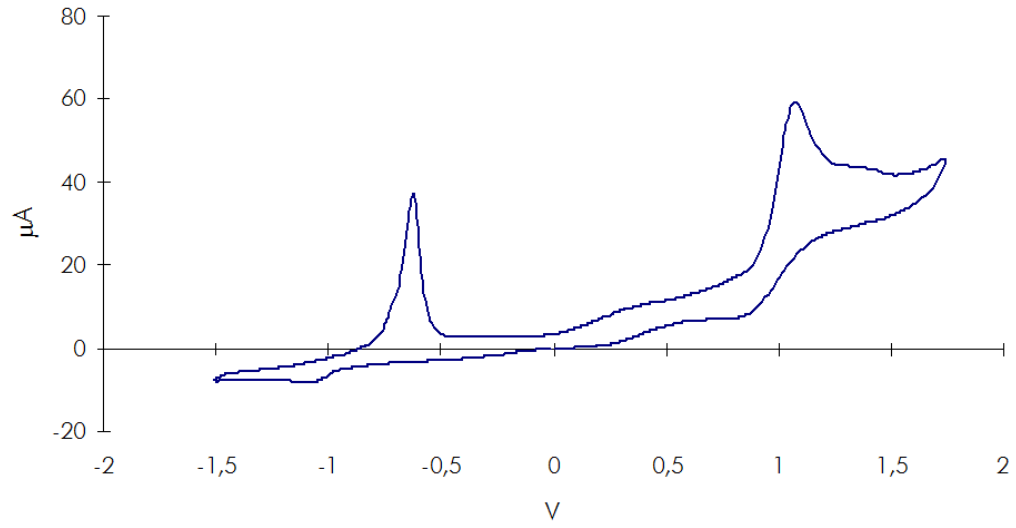

Figure SI18: CV trace of an acetonitrile solution of **5** (10^{-4} M) at a scan rate of 100 mV s^{-1} (supporting electrolyte: 0.1 M Bu_4NPF_6; Ar atmosphere) using a three electrode arrangement with Pt as working and counter electrode and a non-aqueous Ag/Ag^+-reference electrode. The potential was internally referred to the Fc/Fc^+ couple.

Table SI13: Parameters of data collection and crystal structure refinement of compounds **2**·$(CHCl_3)_2$, **3** and **4**·MeCN.

	2·$(CHCl_3)_2$	**3**	**4**·MeCN
Empirical formula	$C_{34}H_{34}Cl_6N_4O_2Si$	$C_{32}H_{32}N_4O_2S_2Si$	$C_{19}H_{28}BCuN_8$
Formula weight	771.44	596.83	442.84
T (K)	180(2)	180(2)	200(2)
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/c$	$P2_1/n$
Unit cell dimens.			
a (Å)	7.1083(6)	7.2839(4)	7.8880(6)
b (Å)	10.0939(9)	20.7778(13)	34.301(2)
c (Å)	13.4480(13)	10.4718(7)	8.8321(7)
α (°)	92.222(7)	90	90
β (°)	96.813(7)	102.342(5)	112.025(6)
γ (°)	100.341(7)	90	90
V (Å^3)	940.74(15)	1548.21(17)	2215.3(3)
Z / D_c (g/cm^3)	1 / 1.36	2 / 1.28	4 / 1.33
μ (mm^{-1})	0.5	0.2	1.1
F(000)	398	628	928
Crystal size (mm)	0.30×0.20×0.10	0.50×0.11×0.03	0.30×0.12×0.04
θ range (°)	2.5-26.0	2.8-26.0	2.4-26.0
Reflns collected	16662	11770	17010
Unique reflns/R_{int}	3705 / 0.0447	3026 / 0.0327	4355 / 0.0592
Completeness to θ_{max}	99.9%	99.8%	100%
Refinement	Full matrix least-squares on F^2		
Data / restraints / parameters	3705 / 13 / 245	3026 / 0 / 190	4355 / 0 / 274
Goodness-of-fit on F^2	1.041	1.027	1.024
$R1$ / $wR2$ [$I > 2\sigma(I)$]	0.0464 / 0.0649	0.0340 / 0.0798	0.0394 / 0.0935
$R1$ / $wR2$ (all data)	0.1059 / 0.1141	0.0460 / 0.0845	0.0642 / 0.1046
Largest diff. peak and hole, eÅ^{-3}	0.351 / -0.334	0.240 / -0.161	0.339 / -0.625

Table SI14: Parameters of data collection and crystal structure refinement of compounds **5**·(ferrocene)$_2$, **5**·toluene and **5**·(toluene)$_4$.

	5·(ferrocene)$_2$	**5**·toluene	**5**·(toluene)$_4$
Empirical formula	$C_{82}H_{96}B_2Cu_2Fe_2N_{16}O_2Si$	$C_{69}H_{84}B_2Cu_2N_{16}O_2Si$	$C_{90}H_{108}B_2Cu_2N_{16}O_2Si$
Formula weight	1626.24	1346.31	1622.73
T (K)	180(2)	100(2)	180(2)
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1
Unit cell dimens.			
a (Å)	10.2646(6)	11.0543(10)	11.3293(7)
b (Å)	11.0643(7)	17.5799(15)	13.7572(8)
c (Å)	18.1798(11)	18.9632(15)	15.5010(10)
α (°)	98.762(5)	97.434(69	80.946(5)
β (°)	96.679(5)	90.778(7)	74.970(5)
γ (°)	90.083(5)	105.074(7)	73.416(5)
V (Å^3)	2026.4(2)	3524.2(5)	2227.2(29
Z / D_c (g/cm^3)	1 / 1.33	2 / 1.27	1 / 1.21
μ (mm^{-1})	0.9	0.7	0.5
F(000)	850	1416	858
Crystal size (mm)	0.35×0.18×0.12	0.15×0.12×0.05	0.35×0.30×0.05
θ range (°)	2.4-27.0	2.3-25.0	2.6-27.0
Reflns collected	21541	26201	23839
Unique reflns/R_{int}	8836 / 0.0384	12351 / 0.0883	9727 / 0.0428
Completeness to θ_{max}	99.9%	99.6%	99.9%
Refinement	Full matrix least-squares on F^2		
Data / restraints / parameters	8836 / 0 / 497	12351 / 0 / 859	9727 / 15 / 581
Goodness-of-fit on F^2	1.034	0.906	1.034
$R1$ / $wR2$ [$I > 2\sigma(I)$]	0.0387 / 0.0914	0.0528 / 0.1252	0.0435 / 0.0987
$R1$ / $wR2$ (all data)	0.0604 / 0.0992	0.1043 / 0.1253	0.0696 / 0.1083
Largest diff. peak and hole, eÅ^{-3}	0.415 / -0.490	0.510 / -0.560	0.298 / -0.250