

Spectroscopic Studies of Bridge Contributions to Electronic Coupling in a Donor-Bridge-Acceptor Biradical System

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NN (Nitronyl Nitroxide)

N	0.00000000	0.00000000	0.00000000
O	1.26600649	0.00000000	0.00000000
C	-0.80361050	1.28737815	0.00000000
C	-2.25293051	0.74785484	-0.28548649
N	-2.11113473	-0.71154212	0.10511508
O	-3.11391276	-1.47674372	0.21406831
C	-0.81367059	-1.05887989	0.15259745
H	-0.46545611	-2.07133610	0.29685217
C	-0.61472952	1.89207480	1.40366162
H	0.33839997	2.37521917	1.45857682
H	-1.38837502	2.60709993	1.59104281
H	-0.66297810	1.11405146	2.13663621
C	-0.21988147	2.23969950	-1.06016247
H	-0.87284194	3.07818717	-1.18458534
H	0.74264929	2.58142383	-0.74132234
H	-0.12387395	1.72116500	-1.99118585
C	-3.38184991	1.38032815	0.54944974
H	-3.32447944	2.44635351	0.47734869
H	-4.32889952	1.04820156	0.17838511
H	-3.27654948	1.08587492	1.57273324
C	-2.64756333	0.74065737	-1.77404725
H	-3.60672320	0.27994005	-1.88652785
H	-2.69028992	1.74646466	-2.13657469
H	-1.91986965	0.19056655	-2.33329852

NN-Ph

N	0.00000000	0.00000000	0.00000000
C	1.36584781	0.00000000	0.00000000
C	2.22480970	1.18698772	0.00000000
C	3.62660095	1.06221438	-0.12730736
C	4.43513877	2.19661816	-0.12864235
C	3.87716674	3.47030796	0.00012196
C	2.49287947	3.60214465	0.12882855
C	1.66807770	2.47950793	0.12738082
H	0.59486055	2.58533670	0.21652065
H	2.04552514	4.58856016	0.22935908
H	4.51494712	4.35163204	0.00015710
H	5.51197109	2.08005114	-0.22911384
H	4.06262112	0.07587126	-0.21648309
N	1.79283772	-1.29741313	0.00010270

S3

C	0.65228518	-2.26527792	-0.21017368
C	-0.56281664	-1.38596033	0.21028596
O	-0.78388678	0.99980951	-0.00745368
O	2.98759909	-1.72943517	0.00741774
C	-0.92185718	-1.47121565	1.70536750
H	-1.39783550	-2.42832061	1.94180250
H	-1.62367465	-0.66433574	1.93705106
H	-0.04002808	-1.35126485	2.34285546
C	-1.82636586	-1.55055129	-0.63502402
H	-2.24878312	-2.55012602	-0.48440835
H	-2.56360723	-0.80669973	-0.32321110
H	-1.63587068	-1.40736910	-1.70112876
C	0.89091427	-3.51693657	0.63515757
H	0.07343457	-4.23061414	0.48461096
H	0.96743935	-3.29119859	1.70125117
H	1.82790561	-3.98477499	0.32332118
C	0.68352900	-2.63301421	-1.70525212
H	0.52176061	-1.75790717	-2.34276049
H	1.66937311	-3.04739378	-1.93694056
H	-0.07678741	-3.38437316	-1.94166034

NN-Ph(OMe)

N	0.00000000	0.00000000	0.00000000
C	1.36574550	0.00000000	0.00000000
C	2.22494273	1.18318435	0.00000000
C	3.62195009	1.06403158	-0.12951008
C	4.44334329	2.19389581	-0.12465913
C	3.87174282	3.46805096	0.00804214
C	2.46856403	3.60134332	0.11360942
C	1.65606302	2.47053373	0.12011954
H	0.58169253	2.55704791	0.19368635
H	4.06361882	0.08016806	-0.21837479
N	1.79003671	-1.29961636	-0.00325347
C	0.64917438	-2.26337119	-0.22404724
C	-0.56520787	-1.38508246	0.19956613
O	-0.78598397	1.00136363	0.00449348
O	2.98428941	-1.73358621	0.00308482
C	-0.92881599	-1.48323369	1.69287895
H	-1.40372239	-2.44322282	1.91946997
H	-1.63231920	-0.67920481	1.92942222
H	-0.04873858	-1.36771076	2.33363455
C	-1.82676625	-1.54264775	-0.65051241
H	-2.24977402	-2.54360585	-0.51047376
H	-2.56501884	-0.80181731	-0.33407384
H	-1.63308917	-1.38970153	-1.71472204

S4

C	0.88267392	-3.52209622	0.61242044
H	0.06426948	-4.23328797	0.45474437
H	0.95713071	-3.30452093	1.68039335
H	1.81963824	-3.98930060	0.29940370
C	0.68267191	-2.62063169	-1.72173978
H	0.52394997	-1.74026356	-2.35267476
H	1.66811261	-3.03517611	-1.95465593
H	-0.07889286	-3.36853344	-1.96457175
C	5.94105444	2.06484407	-0.26791997
H	6.46450408	2.51175915	0.58583447
H	6.23381809	1.01311374	-0.34023230
H	6.30057260	2.58819539	-1.16187382
O	1.98746277	4.87928368	0.18476392
O	4.71106059	4.54872770	-0.05182398
C	0.58036213	5.05984139	0.25232767
C	4.70864863	5.45474871	1.05555876
H	0.41840698	6.14008104	0.27989059
H	0.07650356	4.63813037	-0.62778880
H	0.15472343	4.60473836	1.15739170
H	5.53872927	6.14425504	0.87851296
H	4.88118137	4.91967836	1.99998393
H	3.76983844	6.01228759	1.11999687

Tp^{Cum,Me}Zn(SQ-NN)

C	0.00000000	0.00000000	0.00000000
N	1.35080933	0.00000000	0.00000000
N	1.80956289	1.27688598	0.00000000
C	0.74158364	2.07932507	-0.00476893
C	-0.43892762	1.31856046	0.00070037
B	2.35036687	-1.18376332	-0.04334704
N	3.28315603	-1.09429565	1.18629099
N	4.03849684	0.01660377	1.37035619
C	4.77241897	-0.18220096	2.46820113
C	4.48871874	-1.44324288	3.01990689
C	3.53655787	-1.98858028	2.16733931
Zn	3.88502347	1.47998820	-0.13466157
N	3.98636904	0.03023764	-1.58772158
N	3.21485321	-1.06262991	-1.34050587
C	3.34097136	-1.94161423	-2.35639306
C	4.21809743	-1.41419846	-3.29695433
C	4.59272880	-0.17319073	-2.76294209
O	3.60793829	3.43512319	-0.86765985
C	4.55711957	4.20687033	-0.51782274
C	4.61672836	5.59309732	-0.89586310
C	5.67990263	6.34951591	-0.47118021
C	6.74098784	5.80748396	0.35137255

S5

C	6.70091313	4.46228974	0.73438727
C	5.63525400	3.63785381	0.31696321
C	7.83227435	6.66756131	0.76872312
N	8.87008566	6.30369358	1.59164089
C	9.70932557	7.48850894	2.00232192
C	9.37445123	8.49275956	0.86288848
N	8.02273974	7.98426254	0.42134804
O	9.07381246	5.17641105	2.13707159
O	7.30069761	8.71392159	-0.32566569
C	9.25034501	9.95710713	1.28514453
C	10.29081737	8.38054600	-0.37011755
C	11.17418636	7.06102419	2.10045141
C	9.19492241	7.91383230	3.39044087
C	3.50717337	6.15410613	-1.74435877
O	5.53401298	2.39363921	0.62628533
H	5.26350636	0.57657067	-3.16335479
H	4.53684384	-1.86183656	-4.22732067
H	2.79971333	-2.87779444	-2.33861650
H	1.76030032	-2.22971529	-0.05286612
H	3.02547952	-2.94173763	2.18821330
H	4.91390374	-1.89284179	3.90601748
H	5.46312766	0.58590516	2.79088615
H	-0.54918295	-0.93188813	-0.00179748
H	-1.45970258	1.67353885	0.00250384
H	0.88138171	3.15219944	-0.02175277
H	7.48183794	4.03277737	1.34607780
H	5.74029608	7.39372160	-0.75125369
H	2.53914088	6.06364033	-1.23524515
H	3.68170898	7.20921382	-1.97600036
H	3.41245663	5.59778119	-2.68516655
H	10.22501158	10.33393344	1.61435033
H	8.91533787	10.54990343	0.43061527
H	8.52937873	10.09674050	2.09391595
H	9.84200565	8.95412057	-1.18679683
H	11.28416654	8.78964994	-0.15957845
H	10.40236492	7.34293999	-0.70095563
H	11.79381113	7.91551437	2.39408822
H	11.55416667	6.65940602	1.15825411
H	11.26907733	6.28118014	2.85993821
H	8.14459420	8.22090192	3.35756564
H	9.78926510	8.74080215	3.79202366
H	9.28054432	7.05887950	4.06795688

Tp^{Cum,Me}Zn(SQ-1,4-Ph-NN)

C	0.00000000	0.00000000	0.00000000
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N	1.35093200	0.00000000	0.00000000
N	1.81015975	1.27653274	0.00000000
C	0.74241864	2.07923910	-0.00474521
C	-0.43839041	1.31867451	0.00061243
B	2.35245849	-1.18129843	-0.04021307
N	3.28339938	-1.08650936	1.19129828
N	4.03960977	0.02407501	1.37395145
C	4.76572247	-0.17005387	2.47788742
C	4.47592343	-1.42701173	3.03517350
C	3.52842922	-1.97533483	2.17926677
Zn	3.88987870	1.48195602	-0.13445636
N	3.98607554	0.03211951	-1.58783461
N	3.21773276	-1.06218646	-1.33661310
C	3.34804882	-1.94539317	-2.34823146
C	4.22467385	-1.41952561	-3.29008701
C	4.59474779	-0.17494466	-2.76125629
O	3.60733676	3.44952726	-0.78697351
C	4.57094388	4.21249999	-0.44066789
C	4.61114830	5.61234445	-0.76012004
C	5.69002738	6.34966514	-0.32950168
C	6.78185518	5.78175647	0.41721940
C	6.76191310	4.42754895	0.72913823
C	5.68127393	3.60830262	0.32402443
C	7.90529382	6.64399439	0.83463833
C	7.71616538	8.00728492	1.13546969
C	8.76526360	8.81979485	1.54504929
C	10.07420698	8.29870213	1.66662281
C	10.27534261	6.93216915	1.35993087
C	9.21324981	6.13448132	0.95718707
C	11.18386390	9.14510135	2.09516788
N	12.48605228	8.75158320	2.23574609
C	13.32746150	9.81600165	2.89906548
C	12.46633002	11.08526428	2.62802725
N	11.10195421	10.46895637	2.42811109
O	12.98342924	7.60202468	2.02470852
O	10.07264802	11.21350538	2.42858234
C	12.39862176	12.09860573	3.77134636
C	12.79996390	11.80833808	1.30974366
C	14.72383196	9.81640184	2.27590677
C	13.41911249	9.41586370	4.38343558
C	3.47907635	6.20196395	-1.55683304
O	5.59032600	2.35696058	0.59406696
H	5.26365492	0.57500661	-3.16448351
H	4.54589615	-1.87036091	-4.21805001
H	2.80963884	-2.88309778	-2.32687262
H	1.76524449	-2.22892423	-0.04666905
H	3.01544958	-2.92739893	2.20226326
H	4.89414181	-1.87231946	3.92673746
H	5.45628211	0.59799491	2.80073667
H	-0.54934226	-0.93181570	-0.00152349

H	-1.45912525	1.67379867	0.00247279
H	0.88288134	3.15198773	-0.02122864
H	7.54955549	3.96999908	1.32073909
H	5.74063989	7.40322398	-0.59447865
H	2.52417034	6.08190117	-1.02961566
H	3.63943000	7.26806695	-1.74653028
H	3.36536569	5.68758635	-2.51914016
H	9.40742298	5.09624670	0.70133407
H	11.27200767	6.51670674	1.43083181
H	6.71891067	8.43639058	1.08293878
H	8.58676854	9.85932556	1.78667349
H	13.38033776	12.56194251	3.91907639
H	11.67741684	12.87826438	3.51426297
H	12.07995994	11.64426466	4.71238658
H	12.00992300	12.53746799	1.10631724
H	13.75534173	12.33765028	1.38349286
H	12.84920733	11.11236139	0.46619465
H	15.34457109	10.58435086	2.75055142
H	14.69879186	10.00186792	1.19962068
H	15.18768190	8.84032726	2.43760929
H	12.43418543	9.39731859	4.86079352
H	14.06416697	10.10568631	4.93677393
H	13.84734303	8.41076318	4.44344994

$\text{Tp}^{\text{Cum,Me}}\text{Zn}(\text{SQ-2,5-TP-NN})$

N	0.00000000	0.00000000	0.00000000
C	1.36113613	0.00000000	0.00000000
N	1.80804549	1.29013112	0.00000000
C	0.67008456	2.26123138	0.21421469
C	-0.55875131	1.38492112	-0.20352110
C	2.17705100	-1.17029449	0.00109451
C	3.56891797	-1.22267976	0.00732580
C	4.06519525	-2.53600969	0.00242183
C	3.07639381	-3.51886251	-0.00598477
C	3.23814739	-4.96126061	-0.00690011
C	4.56933079	-5.51605092	0.00351290
C	4.81353599	-6.86742843	0.00587708
C	3.69147344	-7.76790297	0.00036670
C	2.31779854	-7.22194595	-0.01112698
C	2.14034249	-5.82552615	-0.01569481
O	3.82538671	-9.03500038	0.00062206
Zn	1.95950385	-10.01098021	-0.00050845
O	1.35372465	-8.07295377	-0.02155293
C	6.20037587	-7.45098329	0.01483685
O	3.01650464	1.67916351	0.01870828
C	0.91357359	3.51113962	-0.63285034

S8

C	0.70349644	2.62967532	1.70893554
C	-1.81537137	1.54963534	0.65262554
C	-0.92689083	1.48021643	-1.69584134
O	-0.74056246	-1.03212101	-0.02194376
N	1.58337854	-11.23948535	1.60464718
N	1.09941435	-12.46597754	1.26991238
C	0.89320249	-13.18950980	2.38994885
C	1.25060884	-12.41987916	3.49088068
C	1.67732748	-11.20375288	2.93888669
B	0.85170762	-12.87487851	-0.21864583
N	-0.16247262	-11.88911505	-0.84355045
N	0.13320995	-10.56659001	-0.88741096
C	-0.91594631	-9.94519015	-1.43173473
C	-1.91612343	-10.87667962	-1.75869509
C	-1.39210146	-12.10119157	-1.36278209
N	2.19055080	-12.77183060	-0.99183824
N	2.84617450	-11.58594483	-1.05742752
C	3.97810830	-11.79844455	-1.73419043
C	4.06456452	-13.14387632	-2.12804880
C	2.90487606	-13.72486828	-1.62926009
H	2.04348222	-10.31232918	3.43259376
H	1.20773748	-12.69855720	4.53399081
H	0.50780340	-14.19795785	2.32530020
H	0.43016056	-13.99873954	-0.25961518
H	-1.80368484	-13.10035785	-1.41235169
H	-2.87820390	-10.68814337	-2.21362180
H	-0.89334386	-8.86959343	-1.54867126
H	2.54014716	-14.74186372	-1.68128082
H	4.85309716	-13.62387285	-2.69005202
H	4.66651706	-10.97843384	-1.89051858
H	1.12073776	-5.44938987	-0.02467475
H	5.41862670	-4.83856873	0.00987545
H	6.36928773	-8.07457919	-0.87213077
H	6.96302316	-6.66597067	0.03779522
H	6.34439405	-8.10601248	0.88285132
H	5.12664447	-2.75673383	0.00545429
H	4.17296090	-0.32452085	0.01116839
H	0.10923113	4.23745021	-0.47286408
H	1.86078372	3.96472735	-0.32977041
H	0.97596247	3.28586657	-1.69998411
H	1.68901975	3.04515137	1.93993078
H	-0.05784862	3.37971500	1.94585189
H	0.54415920	1.75461678	2.34708597
H	-2.24684090	2.54508892	0.50128332
H	-1.61490316	1.41178852	1.71759083
H	-2.55060930	0.79940275	0.34994226
H	-0.05020465	1.35272978	-2.33889265
H	-1.39263128	2.44406610	-1.92486414
H	-1.63898707	0.68254503	-1.92799742
S	1.48235328	-2.78277294	-0.01059912

Tp^{Cum,Me}Zn(SQ-2,5-Xyl-SQ)

N	0.00000000	0.00000000	0.00000000
C	1.36315878	0.00000000	0.00000000
N	1.81642844	1.27636757	0.00000000
C	0.68150505	2.27013199	0.13237194
C	-0.55118000	1.38477248	-0.24727072
C	2.18392342	-1.21468225	0.07566265
C	3.28420825	-1.44614954	-0.77985033
C	4.00288272	-2.62731035	-0.58791023
C	3.67000543	-3.59549847	0.37681997
C	2.54868142	-3.36551877	1.21037742
C	1.83383871	-2.17910755	1.03296441
C	4.51626516	-4.81449495	0.46157942
C	5.94734898	-4.65951182	0.46082113
C	6.82005470	-5.72358608	0.51085012
C	6.27304815	-7.04971860	0.55493008
C	4.80800786	-7.23179939	0.54984551
C	3.96995217	-6.08783051	0.50450692
O	6.99949080	-8.10128880	0.59399915
Zn	5.85731584	-9.84667203	0.63722803
O	4.36830231	-8.43631251	0.57377845
C	8.31563715	-5.55876036	0.52741263
O	3.02167747	1.66560777	0.09216602
C	0.95564342	3.46461461	-0.78299431
C	0.70427086	2.72757183	1.60212793
C	-1.80535175	1.58476365	0.60544548
C	-0.93037739	1.42478371	-1.73923006
O	-0.76070763	-1.01409687	0.01458880
N	6.07953403	-11.06339337	2.27845770
N	6.23987910	-12.38083072	1.97911164
C	6.38175948	-13.08742370	3.11970757
C	6.31314304	-12.21318503	4.19819145
C	6.12282800	-10.95425107	3.61132513
B	6.24369169	-12.89589592	0.50316393
N	4.89630749	-12.52308516	-0.15864643
N	4.52967660	-11.22020413	-0.24152577
C	3.32464198	-11.18514194	-0.81626877
C	2.89503196	-12.48715133	-1.12387002
C	3.92798608	-13.30584051	-0.68373521
N	7.38883133	-12.19178904	-0.26679047
N	7.40450514	-10.83895618	-0.36676248
C	8.51127989	-10.50613891	-1.03655571
C	9.23134520	-11.65908504	-1.39024366
C	8.47895494	-12.70789085	-0.87536853
H	6.01595466	-9.98365642	4.07927259
H	6.38958417	-12.45286566	5.24902837
H	6.52106567	-14.15931113	3.08403050

H	6.40312829	-14.08621464	0.49590881
H	4.04190631	-14.38130920	-0.70601756
H	1.97020108	-12.78915496	-1.59457784
H	2.83587600	-10.23149901	-0.96677005
H	8.64113513	-13.77712591	-0.89764754
H	10.16148717	-11.72157904	-1.93700032
H	8.73045683	-9.46197441	-1.21687316
H	2.89697819	-6.24817630	0.46996590
H	6.34829624	-3.64799313	0.44419010
H	8.77570995	-6.06281700	-0.33195753
H	8.59931124	-4.50180101	0.50315369
H	8.75218757	-6.01844620	1.42283405
H	0.97084673	-1.99088493	1.66552349
H	4.84383206	-2.82717687	-1.24879471
H	0.17244702	4.22125811	-0.66333709
H	1.91624872	3.90586968	-0.50431744
H	1.00904021	3.18003867	-1.83641434
H	1.69050610	3.14923548	1.81657245
H	-0.05533424	3.49392941	1.78633102
H	0.53419404	1.89257933	2.28934269
H	-2.23739745	2.57360411	0.41625250
H	-1.60274292	1.48945597	1.67459181
H	-2.54011418	0.82228482	0.33422933
H	-0.06039268	1.27015492	-2.38536219
H	-1.39634428	2.38000322	-2.00157093
H	-1.64602361	0.62017238	-1.93368718
C	3.66067280	-0.50863480	-1.89990676
C	2.10992647	-4.31476714	2.30461305
H	2.80459737	-0.32321829	-2.56260214
H	3.98068903	0.46219449	-1.50591839
H	4.46505582	-0.93499765	-2.50725490
H	2.95821587	-4.82840612	2.76687996
H	1.56775407	-3.76984984	3.08481209
H	1.43245914	-5.09072139	1.92491694

NN-Ph E(UB+HF+LYP)=-765.46286924 a.u.

NN-Ph(OMe) E(UB+HF+LYP)=-1033.82092507 a.u.

Tp^{Cum,Me}Zn(SQ-NN) E(UB+HF+LYP)=-3435.63851903 a.u.

Tp^{Cum,Me}Zn(SQ-1,4-Ph-NN) E(UB+HF+LYP)=-3666.69346056 a.u.

Tp^{Cum,Me}Zn(SQ-2,5-TP-NN) E(UB+HF+LYP)=-3987.45443448 a.u.

Tp^{Cum,Me}Zn(SQ-2,5-Xyl-SQ) E(UB+HF+LYP)=-3745.32089783 a.u.