

Supporting Information for: Complex Materials
for Molecular Spintronics Applications: Cobalt
bis(dioxolene) Valence Tautomers, from
Molecules to Polymers

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Optimized atomic structures (angstrom) and total energies (hartree) of molecular VT compounds for both LS and HS configurations.

A. Valence Tautomeric Coordination Compounds

LS-Co(III) - Etot = -314.1647 Hartree

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C	7.764104820	12.412580219	8.888008510
H	7.669429566	11.769099483	9.775620803
H	7.703884280	11.752766005	8.009732446
H	6.894240781	13.080545359	8.866022585
C	20.281618969	15.580456435	9.047831412
H	20.366048889	16.250939481	8.179590579
H	20.354641445	16.212429647	9.945553010
H	21.150371980	14.910656777	9.039221902
C	14.009764859	14.010613044	2.871833887
C	14.013621944	14.011669674	4.296144863
H	10.318484763	11.419401934	8.910334870
H	17.730446530	16.579723119	9.050017191
C	13.993216195	15.217986579	5.009781878
C	14.000750053	15.177827009	6.395425744
C	14.039718966	12.806223491	5.010675350
C	14.043705328	12.848601589	6.395854789
N	14.024824216	14.013317762	7.069273164
H	13.972037065	16.172787170	4.488848172
H	13.987274200	16.078908064	7.004571658
H	14.055762061	11.850357251	4.491691882
H	14.060194974	11.948994605	7.006700990
Co	14.020646098	14.004287749	9.005711322
O	12.682158652	12.669704615	8.984606438
O	12.630006942	15.278586528	9.007679366
O	15.362641584	15.335550295	9.021785635
O	15.408770812	12.726654950	9.002877360
C	11.445143579	14.661966951	8.977814898
C	11.472979469	13.235447473	8.960467155
C	10.276963278	12.509343587	8.923739729
C	10.218788992	15.356158039	8.966466943
C	10.209777719	16.855987976	9.001921177
C	9.050774713	14.594917661	8.930161134
C	9.056286196	13.184960851	8.910380509
C	16.595481778	13.339532805	9.002594531
C	16.570640951	14.766548857	9.018852906

C	17.768697678	15.489769256	9.032364719
C	17.820449465	12.642321991	8.985837602
C	17.829831324	11.142144628	8.956457839
C	18.990168493	13.401437086	8.997381728
C	18.987771746	14.811235390	9.024568503
H	10.749513279	17.282585376	8.143377470
H	10.717841019	17.235430205	9.901199294
H	9.185117714	17.246651780	8.994895097
H	8.090593966	15.115483262	8.918778561
H	17.315959040	10.719215377	9.832536797
H	17.298813330	10.755268170	8.073866721
H	18.855514168	10.754159668	8.938262080
H	19.949284545	12.878809904	8.985460720
C	13.986554074	15.166741659	11.612694785
C	13.983716131	15.210643343	12.998405917
C	14.028963040	12.837963479	11.616936516
C	14.029056574	12.799706039	13.003129372
N	14.011549751	14.000914045	10.940677909
C	14.007497421	14.006586408	13.716037377
C	14.010841366	14.009957903	15.141332837
H	13.969078141	16.066168847	11.001379648
H	13.964616193	16.167647639	13.515330303
H	14.042146066	11.935931524	11.009155601
H	14.046408695	11.845364973	13.524713766
N	14.008339940	14.009141491	1.708436573
N	14.016556917	14.014731540	16.304866471

 HS-Co(II) - Etot = -313.1335 Hartree

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C	7.589915852	12.427418815	8.889185306
H	7.479744902	11.785578352	9.775907042
H	7.528803511	11.768595595	8.010459432
H	6.730919685	13.108834001	8.859145462
C	20.448460542	15.571588576	9.043513555
H	20.540699883	16.242954619	8.177114712
H	20.529165313	16.200102569	9.942859209
H	21.307155810	14.889140965	9.033432751
C	14.008624061	14.011079505	2.614332595
C	14.015198986	14.009857202	4.039100629
H	10.135748939	11.409606905	8.903728458
H	17.903339399	16.591860459	9.024433092
C	14.006614256	15.216415389	4.754310377
C	14.014762589	15.165875489	6.140828361
C	14.030242104	12.802890286	4.753546511

C	14.035166135	12.851132755	6.140074367
N	14.028660180	14.008266574	6.822123983
H	13.992576716	16.172601305	4.235955395
H	14.010017500	16.071869741	6.746393368
H	14.037134743	11.847484432	4.233091909
H	14.042427468	11.945879983	6.746284168
Co	14.019656067	14.002595304	8.960810840
O	12.493917355	12.652996210	8.906408195
O	12.439707919	15.283419790	9.004314818
O	15.544536901	15.350299627	9.015625449
O	15.598137943	12.718719880	8.922308332
C	11.291912752	14.674280131	8.963966905
C	11.318972524	13.212458495	8.931879184
C	10.101674552	12.499886680	8.919926857
C	10.044603582	15.362008082	8.960072688
C	10.029707859	16.860682105	8.986765017
C	8.887970794	14.601565803	8.938296961
C	8.892411176	13.179593514	8.917728420
C	16.745649457	13.327555242	8.969021008
C	16.719017725	14.789613398	8.997698082
C	17.936439515	15.501515384	9.011882348
C	17.992485726	12.638904688	8.979923080
C	18.006689522	11.140145584	8.958208773
C	19.149044645	13.398956008	9.000810207
C	19.145139564	14.820957134	9.016848931
H	10.568720613	17.281168081	8.125059747
H	10.539387092	17.246231486	9.882137387
H	9.003091182	17.246588942	8.977736090
H	7.922922189	15.113449087	8.939138678
H	17.486238811	10.722167315	9.832701827
H	17.477965951	10.752000292	8.075319445
H	19.033281222	10.754247914	8.947856499
H	20.113926155	12.886754006	9.000293061
C	14.002288434	15.159575492	11.779362323
C	13.996760890	15.209627673	13.165736545
C	14.019736155	12.844983516	11.782284116
C	14.018084624	12.796255557	13.168809742
N	14.014697398	14.001468405	11.099073731
C	14.006786954	14.003815067	13.882145688
C	14.008189532	14.006407369	15.306781043
H	13.998921071	16.064087287	11.172141871
H	13.986725260	16.165858196	13.684659071
H	14.025156210	11.937788676	11.178534450
H	14.026075869	11.840882202	13.688746884
N	14.004468543	14.012130079	1.450791405
N	14.011290714	14.009965184	16.470420283

B. Conjugated Monomers with Valence Tautomeric Functionalization

LS-Co(III) - Etot = -387.7633 Hartree

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C	11.698576122	5.861099366	16.955245232
C	10.597285300	3.951137736	18.697555474
C	10.493166782	6.134560412	17.668891355
C	12.349453918	4.615547862	17.097121199
C	11.778759770	3.691019469	17.967303050
C	9.952884206	5.175977680	18.537687081
O	12.181862752	6.846139029	16.207070729
O	9.970698976	7.347277630	17.497980913
Co	10.932068170	8.266754000	16.170219009
O	9.615987219	9.626154849	16.124876865
O	9.958806900	7.392148363	14.826069689
C	8.797691949	8.017182694	14.637714908
C	6.464258771	9.535521812	14.278203255
C	8.608696108	9.237899987	15.352539195
C	7.822325376	7.554416870	13.730026039
C	6.674877073	8.327298557	13.577247547
C	7.435864774	9.987178515	15.167770155
C	12.882335899	9.705018063	12.711699144
H	14.589501052	11.041039508	12.657493781
C	13.870784613	10.528145614	13.294785754
N	12.045907129	9.199407879	14.905265899
C	13.911641847	10.680607878	14.668101151
C	11.996204053	9.039381676	13.586107988
C	12.973776913	10.021250702	15.471134819
H	11.234105013	8.355209128	13.217201123
C	13.622224544	10.958947257	17.738782202
C	13.435339674	10.924825576	19.108321687
C	12.873534657	10.110825300	16.914700103
C	12.485011803	10.042693834	19.660295663
H	14.011328769	11.573417331	19.765985067
C	11.737885118	9.249107387	18.772982028
N	11.937406233	9.282573902	17.455811659
H	14.341673872	11.648454405	17.301944725
H	14.675553141	11.306743565	15.125394919
C	12.288757641	9.937615422	21.057301836
C	12.141045831	9.840695184	22.254837060
C	12.749618167	9.530493550	11.323840349
C	12.583619052	9.353901040	10.128396482

C	12.390484164	9.126849189	8.751981446
C	12.034661517	8.626179921	6.018614783
C	13.403521816	9.450973101	7.825180946
C	11.181214983	8.551899967	8.284473887
C	11.022345850	8.308136165	6.915841577
C	13.231782547	9.198208547	6.467415394
H	14.319349612	9.892462445	8.208630439
H	10.103888614	7.863283881	6.539709262
H	11.911506398	8.435217393	4.953249109
O	14.168506991	9.468771783	5.504252425
O	10.242639255	8.279105246	9.230790652
C	9.010089661	7.691901067	8.817232691
H	8.464290436	8.351198817	8.123948961
H	8.425378177	7.559944700	9.732893344
H	9.175037423	6.712797631	8.341068863
C	15.395603995	10.054945478	5.928000470
H	15.928976415	9.400930365	6.636300736
H	15.228900321	11.038403342	6.396928331
H	15.999367145	10.176737579	5.023531806
H	12.266048512	2.721686683	18.095366491
H	9.032870323	5.406960825	19.076255652
C	10.068836922	2.926203488	19.664223923
H	10.555576827	3.017653243	20.648968318
H	10.258502452	1.903849233	19.310422933
H	8.988909579	3.040036560	19.825833924
C	13.604742584	4.345223963	16.322698529
H	14.364544531	5.118604543	16.511579683
H	13.413907026	4.366326061	15.238793245
H	14.029723913	3.367366638	16.580907816
H	5.906000207	7.986903214	12.880153401
H	7.311582354	10.923055874	15.713639093
C	8.051546289	6.281840056	12.968541428
H	8.982212847	6.323300613	12.381845094
H	7.217790844	6.078902593	12.284339457
H	8.160339649	5.421044000	13.644617992
C	5.190268612	10.307756706	14.065270717
H	5.303728899	11.362758464	14.345574798
H	4.365314662	9.894517903	14.667087750
H	4.870424984	10.269815389	13.014405883
H	10.960120055	8.568388793	19.116368073
H	12.010862422	9.749485512	23.311025544

 HS-Co(II) - Etot = -387.7390 Hartree

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C	11.698576122	5.861099366	16.955245232
C	10.597285300	3.951137736	18.697555474
C	10.493166782	6.134560412	17.668891355
C	12.349453918	4.615547862	17.097121199
C	11.778759770	3.691019469	17.967303050
C	9.952884206	5.175977680	18.537687081
O	12.181862752	6.846139029	16.207070729
O	9.970698976	7.347277630	17.497980913
Co	10.932068170	8.266754000	16.170219009
O	9.615987219	9.626154849	16.124876865
O	9.958806900	7.392148363	14.826069689
C	8.797691949	8.017182694	14.637714908
C	6.464258771	9.535521812	14.278203255
C	8.608696108	9.237899987	15.352539195
C	7.822325376	7.554416870	13.730026039
C	6.674877073	8.327298557	13.577247547
C	7.435864774	9.987178515	15.167770155
C	12.882335899	9.705018063	12.711699144
H	14.589501052	11.041039508	12.657493781
C	13.870784613	10.528145614	13.294785754
N	12.045907129	9.199407879	14.905265899
C	13.911641847	10.680607878	14.668101151
C	11.996204053	9.039381676	13.586107988
C	12.973776913	10.021250702	15.471134819
H	11.234105013	8.355209128	13.217201123
C	13.622224544	10.958947257	17.738782202
C	13.435339674	10.924825576	19.108321687
C	12.873534657	10.110825300	16.914700103
C	12.485011803	10.042693834	19.660295663
H	14.011328769	11.573417331	19.765985067
C	11.737885118	9.249107387	18.772982028
N	11.937406233	9.282573902	17.455811659
H	14.341673872	11.648454405	17.301944725
H	14.675553141	11.306743565	15.125394919
C	12.288757641	9.937615422	21.057301836
C	12.141045831	9.840695184	22.254837060
C	12.749618167	9.530493550	11.323840349
C	12.583619052	9.353901040	10.128396482
C	12.390484164	9.126849189	8.751981446
C	12.034661517	8.626179921	6.018614783
C	13.403521816	9.450973101	7.825180946
C	11.181214983	8.551899967	8.284473887
C	11.022345850	8.308136165	6.915841577
C	13.231782547	9.198208547	6.467415394
H	14.319349612	9.892462445	8.208630439
H	10.103888614	7.863283881	6.539709262

H	11.911506398	8.435217393	4.953249109
O	14.168506991	9.468771783	5.504252425
O	10.242639255	8.279105246	9.230790652
C	9.010089661	7.691901067	8.817232691
H	8.464290436	8.351198817	8.123948961
H	8.425378177	7.559944700	9.732893344
H	9.175037423	6.712797631	8.341068863
C	15.395603995	10.054945478	5.928000470
H	15.928976415	9.400930365	6.636300736
H	15.228900321	11.038403342	6.396928331
H	15.999367145	10.176737579	5.023531806
H	12.266048512	2.721686683	18.095366491
H	9.032870323	5.406960825	19.076255652
C	10.068836922	2.926203488	19.664223923
H	10.555576827	3.017653243	20.648968318
H	10.258502452	1.903849233	19.310422933
H	8.988909579	3.040036560	19.825833924
C	13.604742584	4.345223963	16.322698529
H	14.364544531	5.118604543	16.511579683
H	13.413907026	4.366326061	15.238793245
H	14.029723913	3.367366638	16.580907816
H	5.906000207	7.986903214	12.880153401
H	7.311582354	10.923055874	15.713639093
C	8.051546289	6.281840056	12.968541428
H	8.982212847	6.323300613	12.381845094
H	7.217790844	6.078902593	12.284339457
H	8.160339649	5.421044000	13.644617992
C	5.190268612	10.307756706	14.065270717
H	5.303728899	11.362758464	14.345574798
H	4.365314662	9.894517903	14.667087750
H	4.870424984	10.269815389	13.014405883
H	10.960120055	8.568388793	19.116368073
H	12.010862422	9.749485512	23.311025544