Electronic communication through molecular bridges
— Supporting Information

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1 Computational Methodology

1.1 Molecular structures and energies

Molecular structures were optimized using Kohn–Sham density functional theory [1] with the BP86 exchange–correlation functional [2,3] in combination with the resolution-of-the-identity ('RI') density fitting technique as implemented in Turbomole 6.0 [4–6], until the norm of the gradient was below 10^{-4} a.u. The convergence criterion in the self-consistent-field algorithm was set to 10^{-7} a.u. for the change in energy. Where explicitly mentioned, the B3LYP functional [7, 8] was employed instead. For the thiophene- and furane-bridged systems, we employed Ahlrichs' def-TZVP basis set, and for all other calculations Ahlrichs' def2-TZVP basis set [9], which both feature a split-valence triple-zeta basis set with polarization functions on all atoms.

Spin-state energy splittings $E_T - E_{BS}$ were obtained by optimizing the molecular structures for each spin state separately. For the diradical based on the alkyne-linked ethene bridge, we first optimized the structure in the triplet state, and then elongated the outermost C–C bond to 1.7 Å and carried out single-point calculations on this structure for both the triplet and the singlet. The artificial elongation was done to prevent open-shell singlet calculations from converging to a closed-shell singlet. For the "opt. + 0.2 Å" calculation, additionally the middle C–C bond was elongated by 0.2 Å and triplet and singlet single-point calculations were carried out subsequently (see below for Cartesian coordinates). Initial guess orbitals for the Broken-Symmetry determinants were obtained from a tool implemented in a local version of Turbomole 5.1.8 [10]. Equation (1) in the main manuscript is based on spin projection. When arguing that KS determinants need not be pure eigenfunctions of the total spin operator $\hat{S}^2$ [11, 12], so that spin projection is not required, instead $-J_{AB} = \frac{1}{2}(E_T - E_{BS})$ would hold. However, accepting one or the other as correct will not change relative values for J_{AB}, so we report trends in $E_T - E_{BS}$.

For the conductance calculations, dithiol molecules were optimized, the thiol groups' hydrogen atoms were stripped off, and the structures were placed between two Au_9 clusters with an sulfur–gold distance of 2.48 Å [13]. Au–Au distances were set to their value in extended gold crystals (2.88 Å). Fock and overlap matrices as required for the subsequent transport calculation (see below) were then obtained from a single-point electronic structure calculation on the Au_9–molecule–Au_9 system using the Gaussian quantum chemistry program package, with the BP86 exchange–correlation functional [2,3] and the LANL2DZ effective core potential (ECP) with matching basis sets of double-zeta quality as implemented in Gaussian [14]

MOs were plotted using Molden [15], with isodensity values of 0.02, and postprocessed with a local postprocessing tool by Gemma C. Solomon, University of Copenhagen. For molecular junctions (Au_9–molecule–Au_9 structures), central subsystem MOs are plotted, which were calculated by solving the secular equation for the central subsystem only [16].

1.2 Electron transport calculations

Transmission functions were obtained by postprocessing output from electronic structure calculations on these finite-size electrode–molecule–electrode systems, using routines written in our laboratory [17, 18]. In the Green's function approach, T_s is calculated from a trace over matrices describing the coupling of a central region [19] to the left and right electrodes, $\mathbf{\Gamma}_{L/R,s}$, and the central system

subblock of the retarded and advanced Green's functions of the electrode–molecule–electrode system $\mathbf{G}^{r/a}_{C,s}$ [20, 21],

$$T_s(E) = tr\left\{\mathbf{\Gamma}_{R,s}(E)\mathbf{G}^{r}_{C,s}(E)\mathbf{\Gamma}_{L,s}(E)\mathbf{G}^{a}_{C,s}(E)\right\}, \quad (1)$$

the advanced Green's function being the complex conjugate of the retarded. $\mathbf{\Gamma}_{X,s}$ and $\mathbf{G}^{r}_{C,s}$ are calculated from the overlap and Fock matrices of a finite-cluster electrode–molecule–electrode system,

$$\mathbf{\Gamma}_{X,s} = -2\mathrm{Im}[(E\mathbf{S}_{XC} - \mathbf{H}_{XC,s})^{\dagger}\,\mathbf{g}_{X,s}\,(E\mathbf{S}_{XC} - \mathbf{H}_{XC,s})] \quad (2)$$

$$\mathbf{G}^{r}_{C,s} = (E\mathbf{S}_{C} - \mathbf{H}_{C,s} + i\tfrac{1}{2}\mathbf{\Gamma}_{R,s} + i\tfrac{1}{2}\mathbf{\Gamma}_{L,s})^{-1}. \quad (3)$$

The Fock and overlap matrices of the electrode–molecule–electrode system are divided into central, left-electrode, and right-electrode regions. $\mathbf{S}_{XC}$ and $\mathbf{H}_{XC,s}$ denote the coupling block of electrode X and molecule in the overlap and Fock matrix, respectively, while the molecule (or "central region") subblocks of these matrices are indicated by the subscript C. The central region consisted of the molecule only (i.e., no gold atoms were included) as we are interested in qualitative trends only.

The Green's function matrices of the isolated electrodes X ($X \in \{L, R\}$) were calculated in the wide-band-limit (WBL) approximation,

$$(\mathbf{g}_X)_{ij} = -i \cdot \pi \cdot \mathrm{LDOS}_{\mathrm{const}} \cdot \delta_{ij}, \quad (4)$$

i.e., the local density of states (LDOS) was assumed to be independent of the energy, and furthermore, the same LDOS value of 0.036 eV^{-1}, obtained from the *s*-band LDOS for bulk gold from DFT calculations [22] was assigned to all basis functions. Although this is a rather crude approximation, it typically works very well for electrode metals such as gold, which feature a comparatively flat LDOS distribution around the Fermi energy (when plotted as a function of energy), and whose conduction properties are dominated by the broad *s* band [23].

Energies were not shifted by the system's Fermi energy.

2 Total energies and Cartesian Coordinates

All coordinates are given in Å; all energies in hartree.

2.1 Alkyne-linked ethene bridge

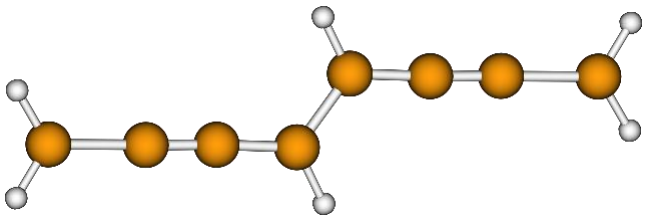


Figure 1: Structure of diradical formed from alkyne-linked ethene bridge. Optimized with KS-DFT(BP86)/def2-TZVP in the triplet state, then both outermost C–C bonds set to 1.7 Å and middle C–C bond elongated by 0.2 Å.

Diradical: BP86/def2-TZVP optimized in the triplet, both outermost C–C bonds set to 1.7 Å

C	-3.478680	0.000015	-2.055614
C	-2.028683	-0.000055	-1.168261
C	-0.976685	-0.000121	-0.513027
C	0.237378	-0.000164	0.189878
C	0.334704	0.000136	1.560143
C	1.548759	0.000093	2.263003
C	2.600731	0.000027	2.918249
C	4.050723	-0.000065	3.805611
H	-4.446098	-0.000385	-1.552558
H	5.018135	-0.001258	3.302590
H	-3.470046	0.000433	-3.145924
H	4.042122	0.001095	4.895900
H	-0.586922	0.000394	2.149888
H	1.159033	-0.000421	-0.399829

Total energy triplet BP86/def2-TZVP: -308.26410796363
Total energy singlet BP86/def2-TZVP: -308.27155859980

Diradical: as above, additionally middle C–C bond elongated by 0.2 Å

C	-3.478613	0.000015	-2.055574
C	-2.028644	-0.000055	-1.168238
C	-0.976666	-0.000121	-0.513017
C	0.237373	-0.000164	0.189874
C	0.348867	0.000180	1.759606
C	1.562898	0.000137	2.462452
C	2.614850	0.000071	3.117686
C	4.064814	-0.000021	4.005031
H	-4.446012	-0.000385	-1.552528
H	5.032207	-0.001214	3.502019
H	-3.469979	0.000433	-3.145863
H	4.056213	0.001139	5.095298
H	-0.572741	0.000438	2.349340
H	1.159011	-0.000421	-0.399821

Total energy triplet BP86/def2-TZVP: -308.23863550288
Total energy singlet BP86/def2-TZVP: -308.25127015421

Junction from optimized dithiol

C	-0.48786662	0.00000000	-0.47822996
C	0.48802910	0.00000000	0.47805833
C	0.25504667	0.00000000	1.86116575

C	−0.25485335	0.00000000	-1.86132424
H	−1.53588206	0.00000000	-0.16398155
H	1.53604156	0.00000000	0.16389671
C	−0.08109894	0.00000000	-3.07504803
C	0.08103780	0.00000000	3.07489221
S	0.00000033	0.00000000	4.75053434
S	0.00000000	0.00000000	-4.75053406
Au	-1.44000000	-0.83137561	8.93943200
Au	1.44000000	-0.83137561	8.93943200
Au	0.00000000	1.66277439	8.93943200
Au	0.00000000	-1.66276561	6.58792200
Au	1.44000000	0.83138439	6.58792200
Au	-1.44000000	0.83138439	6.58792200
Au	-2.88000000	-1.66276561	6.58792200
Au	2.88000000	-1.66276561	6.58792200
Au	0.00000000	3.32554439	6.58792200
Au	-1.44000000	-0.83137561	-8.93943200
Au	1.44000000	-0.83137561	-8.93943200
Au	0.00000000	1.66277439	-8.93943200
Au	0.00000000	-1.66276561	-6.58792200
Au	1.44000000	0.83138439	-6.58792200
Au	-1.44000000	0.83138439	-6.58792200
Au	-2.88000000	-1.66276561	-6.58792200
Au	2.88000000	-1.66276561	-6.58792200
Au	0.00000000	3.32554439	-6.58792200

Total energy BP86/LANL2DZ: -2690.16373165

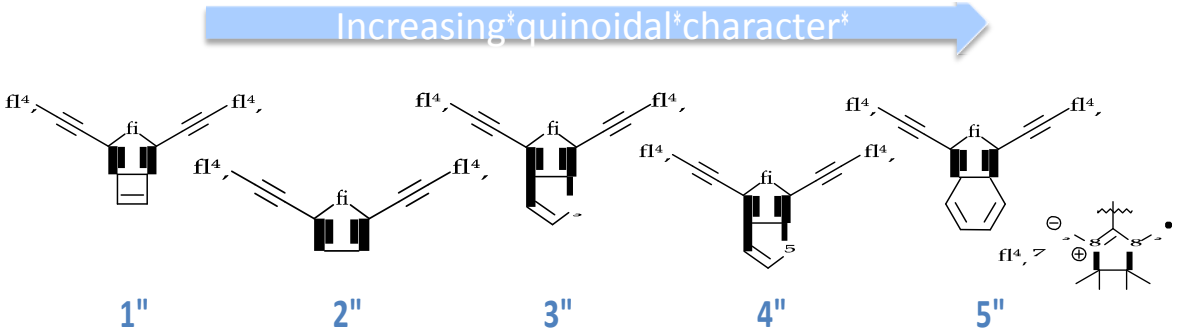
Junction from optimized dithiol, middle C−C bond elongated by 0.2 Å

C	-0.487867	0.000000	-0.478230
C	-0.254853	0.000000	-1.861324
C	-0.081099	0.000000	-3.075048
S	0.000000	0.000000	-4.750534
C	0.630878	0.000000	0.618038
C	0.397896	0.000000	2.001145
C	0.223887	0.000000	3.214871
S	0.142849	0.000000	4.890514
H	-1.535882	0.000000	-0.163982
H	1.678891	0.000000	0.303876
Au	-1.297151	0.831385	6.727901
Au	0.142849	3.325544	6.727901
Au	1.582849	0.831384	6.727901
Au	3.022849	-1.662766	6.727902
Au	0.142896	-1.662738	6.727901
Au	-2.737104	−1.662711	6.727901
Au	-1.297096	−0.831334	9.079411
Au	0.142928	1.662802	9.079411

Au	1.582904	-0.831362	9.079412
Au	-1.440000	0.831384	-6.587922
Au	0.000000	3.325544	-6.587922
Au	1.440000	0.831384	-6.587922
Au	2.880000	-1.662765	-6.587922
Au	-0.000090	-1.662818	-6.587922
Au	-2.880091	-1.662871	-6.587922
Au	-1.440106	-0.831454	-8.939432
Au	-0.000152	1.662722	-8.939432
Au	1.439894	-0.831401	-8.939436

Total energy BP86/LANL2DZ: -2690.14455166

2.2 Furane- and thiophene-bridged systems with fused rings



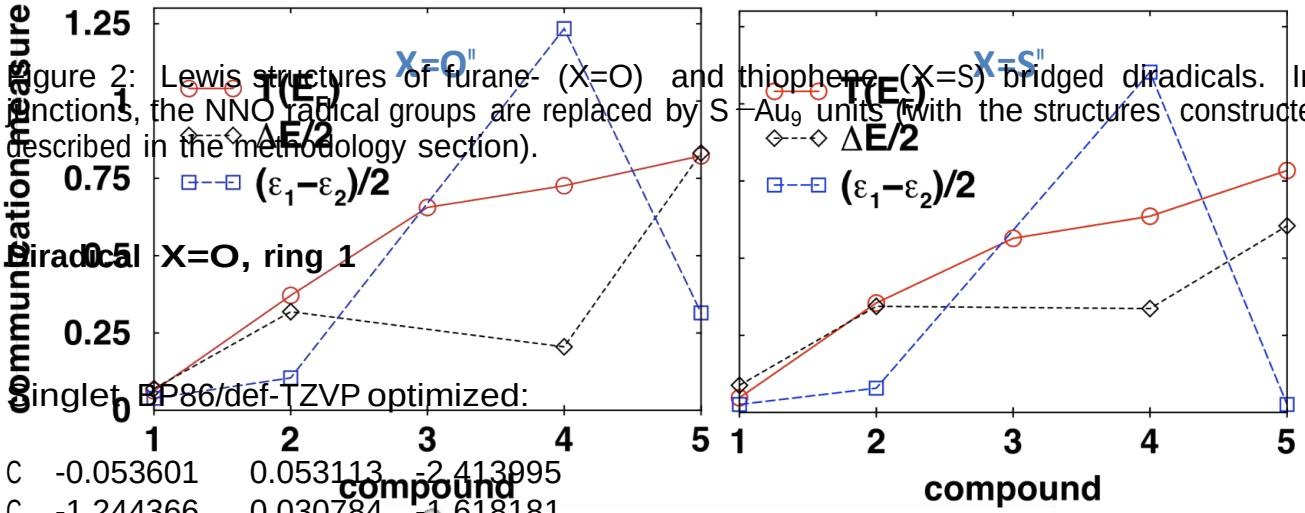


Figure 2: Lewis structures of furane- (X=O) and thiophene (X=S) bridged diradicals. In the junctions, the NNO radical groups are replaced by S–Au_9 units (with the structures constructed as described in the methodology section).

Diradical X=O, ring 1

Singlet, BP86/def-TZVP optimized:

C	-0.053601	0.053113	-2.413995
C	-1.244366	0.030784	-1.618181
C	-0.873276	-0.003844	-0.305943
O	0.542281	-0.003990	-0.234704
C	1.017666	0.031164	-1.569719
C	-1.598281	-0.025693	0.884505
C	-2.316201	-0.052579	1.873947
C	-3.193030	-0.052681	2.953360
C	2.395242	0.022577	-1.783246
C	3.585192	0.023571	-2.064626
C	4.919575	-0.003665	-2.455362
N	-4.530664	0.239165	2.859888
N	-2.261967	-0.343150	-4.250846

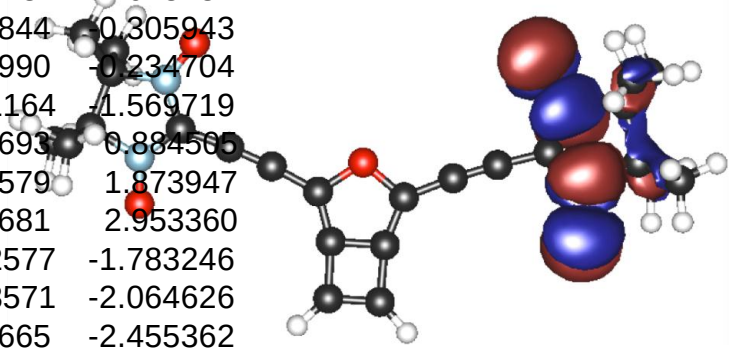


Fig. 2 Lewis structures (top) and trends in different communication measures (middle) for furane and thiophene bridges;, and magnetic MO (bottom) for furane system 1. D$E = E_T - E_{BS}$. Energies in kJ/mol. KS-DFT(BP86).

C	-5.233902	-0.071537	4.175328
C	-4.031747	-0.028735	5.178372
O	-1.712786	-0.663328	4.688729
O	-5.167782	0.550233	1.803498
C	-3.744903	1.368578	5.752711
C	-4.075578	-1.063447	6.298837
C	-5.853417	-1.467884	3.999084
C	-6.327372	0.964688	4.416558
H	-4.521238	1.659337	6.473186
H	-2.778132	1.342935	6.272631
H	-3.692488	2.132443	4.964600
H	-4.909979	-0.842674	6.978972
H	-4.189160	-2.085145	5.918458
H	-3.138949	-1.016673	6.868223
H	-6.534967	-1.442738	3.138239
H	-5.089071	-2.234167	3.812473
H	-6.428384	-1.753641	4.890346
H	-7.055404	0.915815	3.596881
H	-6.847968	0.746904	5.359643
H	-5.931925	1.985988	4.457267
N	5.993615	0.259892	-1.646468
N	5.345144	-0.298240	-3.726313
C	6.836573	-0.018687	-3.864292
C	7.295004	-0.077719	-2.368065
C	7.460138	-1.065174	-4.783334
C	6.944136	1.378650	-4.497665
C	7.685400	-1.485493	-1.887671
C	8.364970	0.934037	-1.969759
O	4.611567	-0.590639	-4.723672
O	5.959554	0.576909	-0.416444
H	7.994449	1.643733	-4.679531
H	6.415297	1.369104	-5.459797
H	6.491362	2.151928	-3.862048
H	8.536033	-0.870772	-4.895871
H	7.322547	-2.085180	-4.406808
H	6.988285	-1.002135	-5.771727
H	8.528580	0.877474	-0.886459
H	9.310281	0.699321	-2.479184
H	8.077075	1.962718	-2.215283
H	7.787582	-1.466837	-0.794599
H	6.924750	-2.233203	-2.150632
H	8.646107	-1.792810	-2.322316
C	-2.055357	0.062749	-2.886802
C	-0.916740	0.082759	-3.647973
H	-3.120599	0.069105	-3.102039
H	-0.708765	0.107576	-4.714378

Total energy singlet BP86/def-TZVP: -1525.47896280713

Triplet BP86/def-TZVP optimized:

C	-0.053428	0.053135	-2.413977
C	-1.244430	0.030821	-1.617991
C	-0.873076	-0.003802	-0.305829
O	0.542370	-0.004000	-0.234607
C	1.017678	0.031190	-1.569528
C	-1.597883	-0.025834	0.884840
C	-2.316081	-0.052914	1.874033
C	-3.193318	-0.052896	2.953215
C	2.395415	0.022707	-1.782743
C	3.585224	0.023854	-2.064510
C	4.919544	-0.003503	-2.455666
N	-4.530788	0.239188	2.859760
N	-2.862130	-0.343092	4.250721
C	-5.233973	-0.071466	4.175271
C	-4.031917	-0.028670	5.178340
O	-1.713026	-0.663307	4.688825
O	-5.167620	0.550274	1.803250
C	-3.744904	1.368590	5.752680
C	-4.075650	-1.063424	6.298830
C	-5.853441	-1.467859	3.999066
C	-6.327369	0.964707	4.416526
H	-4.521276	1.659312	6.473117
H	-2.778149	1.342844	6.272631
H	-3.692390	2.132502	4.964603
H	-4.909967	-0.842748	6.979104
H	-4.189216	-2.085092	5.918398
H	-3.139012	-1.016691	6.868204
H	-6.534950	-1.442626	3.138209
H	-5.089076	-2.234133	3.812458
H	-6.428484	-1.753670	4.890261
H	-7.055326	0.915697	3.596813
H	-6.847951	0.746854	5.359638
H	-5.931995	1.986028	4.457295
N	5.993569	0.259826	-1.646644
N	5.345072	-0.298312	-3.726435
C	6.836557	-0.018750	-3.864368
C	7.295023	-0.077754	-2.368184
C	7.460089	-1.065237	-4.783358
C	6.944132	1.378635	-4.497721
C	7.685400	-1.485508	-1.887673
C	8.364994	0.934037	-1.969792
O	4.611297	-0.590740	-4.723603
O	5.959744	0.577045	-0.416658
H	7.994446	1.643743	-4.679616

H	6.415271	1.369127	-5.459826
H	6.491398	2.151953	-3.862105
H	8.536012	-0.870792	-4.895916
H	7.322571	-2.085222	-4.406819
H	6.988197	-1.002219	-5.771709
H	8.528667	0.877644	-0.886483
H	9.310316	0.699298	-2.479172
H	8.076978	1.962685	-2.215311
H	7.787617	-1.466840	-0.794612
H	6.924752	-2.233238	-2.150604
H	8.646076	-1.792812	-2.322355
C	-2.055290	0.062695	-2.886567
C	-0.916607	0.082836	-3.647795
H	-3.120542	0.069011	-3.101985
H	-0.708738	0.107708	-4.714250

Total energy triplet BP86/def-TZVP: -1525.47890908412

Diradical X=O, ring 2 (= no ring)

Singlet BP86/def-TZVP optimized:

C	-0.031719	0.076230	-2.354919
C	-1.200642	0.059339	-1.570129
C	-0.793823	0.017174	-0.241783
O	0.586532	0.007979	-0.172526
C	1.044685	0.044152	-1.476192
C	-1.538830	-0.004502	0.934140
C	-2.279724	-0.033859	1.907762
C	-3.180935	-0.041362	2.965724
C	2.415324	0.028761	-1.719933
C	3.598424	0.025685	-2.032971
C	4.923758	-0.002916	-2.450700
N	-4.514037	0.261914	2.843203
N	-2.885715	-0.354614	4.267087
C	-5.252242	-0.066127	4.134682
C	-4.076086	-0.042522	5.168719
O	-1.750652	-0.692969	4.728761
O	-5.121120	0.594124	1.775338
C	-3.795768	1.346531	5.765971
C	-4.157064	-1.088782	6.276186
C	-5.870986	-1.457805	3.922522
C	-6.347964	0.970409	4.363161
H	-4.588474	1.634057	6.469818
H	-2.842855	1.309544	6.310256
H	-3.719024	2.118623	4.988030

H	-5.012190	-0.872250	6.931485
H	-4.261413	-2.106155	5.881992
H	-3.239241	-1.050938	6.876104
H	-6.530330	-1.418110	3.045234
H	-5.104314	-2.223933	3.744519
H	-6.469158	-1.754597	4.794711
H	-7.054535	0.936547	3.524230
H	-6.893186	0.740665	5.289276
H	-5.950058	1.989413	4.429069
N	6.014060	0.275934	-1.668259
N	5.323824	-0.313154	-3.726334
C	6.811145	-0.032389	-3.899135
C	7.301035	-0.067613	-2.411821
C	7.418091	-1.091925	-4.814262
C	6.902801	1.355128	-4.556502
C	7.707647	-1.466574	-1.919202
C	8.375935	0.953706	-2.052594
O	4.569434	-0.618825	-4.704260
O	6.003945	0.607282	-0.441106
H	7.948525	1.618742	-4.764925
H	6.353434	1.329235	-5.506718
H	6.462423	2.137894	-3.923751
H	8.491961	-0.899782	-4.948336
H	7.286813	-2.106407	-4.420940
H	6.928937	-1.042354	-5.794932
H	8.567315	0.911429	-0.973222
H	9.309062	0.716397	-2.582845
H	8.077645	1.978113	-2.303698
H	7.834752	-1.430995	-0.829162
H	6.943933	-2.220625	-2.153443
H	8.659253	-1.777421	-2.371076
H	-2.231338	0.076190	-1.908425
H	0.044671	0.106616	-3.436735

Total energy singlet BP86/def-TZVP: -1449.35369086134

Triplet BP86/def-TZVP optimized:

C	-0.029562	0.077323	-2.351826
C	-1.198644	0.059169	-1.566440
C	-0.791208	0.016413	-0.238851
O	0.588931	0.008050	-0.169687
C	1.046423	0.045314	-1.473429
C	-1.536675	-0.005266	0.937244
C	-2.277998	-0.034360	1.910121
C	-3.180896	-0.042303	2.967172
C	2.417483	0.029944	-1.717298

C	3.599826	0.026470	-2.031777
C	4.925166	-0.001895	-2.450763
N	-4.513305	0.262103	2.843291
N	-2.886805	-0.356544	4.268153
C	-5.252880	-0.066134	4.133930
C	-4.077555	-0.042932	5.168724
O	-1.752656	-0.696839	4.730650
O	-5.119214	0.595536	1.775140
C	-3.796463	1.346149	5.765501
C	-4.160248	-1.088780	6.276219
C	-5.871201	-1.457976	3.921385
C	-6.348600	0.970653	4.361760
H	-4.589849	1.634890	6.468081
H	-2.844301	1.308241	6.311049
H	-3.717804	2.117719	4.987201
H	-5.016309	-0.872177	6.930268
H	-4.264150	-2.106086	5.881787
H	-3.243121	-1.050799	6.877092
H	-6.530444	-1.418938	3.044006
H	-5.104094	-2.223760	3.743741
H	-6.469322	-1.754996	4.793552
H	-7.054786	0.937600	3.522480
H	-6.894557	0.740908	5.287420
H	-5.950421	1.989531	4.428262
N	6.015452	0.277860	-1.669113
N	5.323914	-0.312947	-3.726084
C	6.811057	-0.032702	-3.900145
C	7.301903	-0.066795	-2.413121
C	7.415993	-1.093315	-4.815356
C	6.902529	1.354531	-4.558211
C	7.707962	-1.465462	-1.919259
C	8.377301	0.954221	-2.054762
O	4.568860	-0.619136	-4.703374
O	6.006039	0.610005	-0.442206
H	7.948154	1.618209	-4.767017
H	6.352938	1.328470	-5.508276
H	6.462262	2.137385	-3.925501
H	8.490071	-0.903167	-4.950181
H	7.282864	-2.107501	-4.421833
H	6.926230	-1.043211	-5.795715
H	8.569441	0.910922	-0.975558
H	9.309910	0.717142	-2.586059
H	8.078775	1.978818	-2.304846
H	7.836228	-1.428504	-0.829407
H	6.943392	-2.219216	-2.151647
H	8.658836	-1.777620	-2.371664
H	-2.229625	0.075521	-1.904015
H	0.046688	0.108575	-3.433664

Total energy triplet BP86/def-TZVP: -1449.35344796941

Diradical X=O, ring 4

Singlet BP86/def-TZVP optimized:

C	0.100141	-0.020339	-2.281889
C	-1.097203	-0.030792	-1.511838
C	-0.747214	-0.023462	-0.164448
O	0.639805	-0.005483	-0.076590
C	1.155681	-0.003530	-1.362482
C	-1.508502	-0.025409	0.993250
C	-2.258341	-0.040763	1.962245
C	-3.143680	-0.040835	3.031719
C	2.526152	0.000672	-1.560116
C	3.714065	0.012429	-1.863155
C	5.032696	-0.006953	-2.294191
N	-4.484581	0.233907	2.927493
N	-2.818797	-0.317102	4.335355
C	-5.192675	-0.075707	4.240034
C	-3.998296	-0.008453	5.251337
O	-1.666889	-0.615094	4.783897
O	-5.117741	0.525043	1.862469
C	-3.734371	1.397503	5.815684
C	-4.038238	-1.033687	6.380999
C	-5.793061	-1.481448	4.072140
C	-6.300969	0.948465	4.464540
H	-4.518556	1.683711	6.529511
H	-2.770223	1.390022	6.341034
H	-3.688583	2.155248	5.021278
H	-4.882684	-0.818773	7.050554
H	-4.133468	-2.060355	6.009001
H	-3.108370	-0.968395	6.959527
H	-6.469088	-1.472671	3.206666
H	-5.017812	-2.239580	3.897176
H	-6.370161	-1.766733	4.962170
H	-7.020620	0.884903	3.638578
H	-6.827598	0.730807	5.404280
H	-5.918308	1.974758	4.501594
N	6.138620	0.215957	-1.514800
N	5.411498	-0.250684	-3.591719
C	6.898195	0.022537	-3.771625
C	7.409609	-0.101083	-2.296322
C	7.478420	-0.991609	-4.753656
C	6.998367	1.443127	-4.351965
C	7.806374	-1.529841	-1.888790

C	8.503153	0.885343	-1.898334
O	4.636768	-0.486033	-4.574877
O	6.149985	0.475410	-0.270038
H	8.044070	1.704972	-4.562712
H	6.433971	1.477387	-5.293065
H	6.578375	2.194405	-3.669226
H	8.552160	-0.804299	-4.895162
H	7.341164	-2.024748	-4.414500
H	6.974173	-0.882917	-5.721990
H	8.708420	0.782043	-0.825614
H	9.425459	0.664798	-2.454144
H	8.215914	1.925623	-2.089539
H	7.950321	-1.556356	-0.800515
H	7.030172	-2.261094	-2.152441
H	8.747444	-1.825820	-2.371932
C	-0.142042	-0.033263	-3.691959
S	-2.522273	-0.053101	-2.523738
C	-1.480112	-0.051424	-3.960575
H	-1.959713	-0.064191	-4.936254
H	0.632858	-0.033120	-4.455808

Total energy singlet BP86/def-TZVP: -1923.83202632995

Triplet BP86/def-TZVP optimized:

C	-0.140948	-0.054617	-2.620022
C	-1.327033	-0.057961	-1.829314
C	-0.955477	-0.031907	-0.488952
O	0.432094	-0.011284	-0.425371
C	0.928785	-0.025604	-1.718544
C	-1.679331	-0.021718	0.693447
C	-2.353018	-0.022353	1.716161
C	-3.126448	-0.021515	2.869858
C	2.301354	-0.020273	-1.907841
C	3.505759	-0.013866	-2.133065
C	4.867908	-0.019300	-2.401299
N	-4.472222	0.240884	2.908650
N	-2.659557	-0.286109	4.131889
C	-5.031715	-0.070555	4.291335
C	-3.736209	0.014856	5.168151
O	-1.463384	-0.570857	4.454259
O	-5.218334	0.522708	1.916868
C	-3.428868	1.426630	5.694550
C	-3.640027	-1.004612	6.299612
C	-5.628759	-1.484663	4.192891
C	-6.122070	0.941116	4.630705
H	-4.132637	1.706850	6.489824

H	-2.412460	1.432692	6.110086
H	-3.481088	2.181005	4.897486
H	-4.405100	-0.792788	7.059478
H	-3.767586	-2.034123	5.945267
H	-2.650906	-0.928700	6.768375
H	-6.392014	-1.488655	3.402889
H	-4.866303	-2.233999	3.941032
H	-6.105847	-1.772544	5.139390
H	-6.927460	0.864431	3.889183
H	-6.540048	0.722422	5.623499
H	-5.750761	1.972258	4.621526
N	5.856875	0.172928	-1.470470
N	5.419179	-0.219856	-3.641310
C	6.917104	0.054826	-3.606271
C	7.222209	-0.124693	-2.080309
C	7.627693	-0.924111	-4.536778
C	7.093276	1.495598	-4.113779
C	7.555555	-1.570087	-1.674071
C	8.250839	0.839545	-1.497359
O	4.786973	-0.423169	-4.727938
O	5.697262	0.389476	-0.227856
H	8.157388	1.761875	-4.166227
H	6.666137	1.567263	-5.123026
H	6.580012	2.221866	-3.468976
H	8.709581	-0.731440	-4.527371
H	7.451675	-1.968704	-4.255359
H	7.255983	-0.781821	-5.559188
H	8.298194	0.699507	-0.410204
H	9.243329	0.629649	-1.920557
H	7.997203	1.887796	-1.692422
H	7.542763	-1.638019	-0.578149
H	6.823551	-2.285753	-2.072763
H	8.555268	-1.853762	-2.029380
C	-0.408817	-0.087212	-4.025444
S	-2.768787	-0.097998	-2.817199
C	-1.751059	-0.112753	-4.271150
H	-2.247199	-0.140708	-5.238152
H	0.351409	-0.094131	-4.803757

Total energy triplet BP86/def-TZVP: -1923.83186996420

Diradical X=O, ring 5

Singlet BP86/def-TZVP optimized:

C	-0.273924	0.190736	-2.122755

C	-1.444544	0.202340	-1.289986
C	-0.987774	0.133948	0.041947
O	0.390082	0.087271	0.051143
C	0.833869	0.121955	-1.254020
C	-1.688932	0.098561	1.233229
C	-2.415499	0.054585	2.220805
C	-3.289307	0.022244	3.296679
C	2.189737	0.082298	-1.522539
C	3.365200	0.062252	-1.873207
N	-4.634923	0.283007	3.206883
N	-2.954355	-0.278874	4.592508
C	-5.331560	-0.065103	4.514812
C	-4.131990	-0.007195	5.521085
O	-1.795985	-0.572376	5.027542
O	-5.278288	0.586604	2.150207
C	-3.882532	1.387797	6.118375
C	-4.152835	-1.059836	6.625716
C	-5.915842	-1.474058	4.318112
C	-6.450764	0.939897	4.770583
H	-4.666831	1.646973	6.842232
H	-2.915886	1.378740	6.639162
H	-3.848993	2.165220	5.342607
H	-4.996635	-0.872139	7.304139
H	-4.236167	-2.078383	6.229482
H	-3.220970	-0.996050	7.201268
H	-6.596463	-1.453975	3.456434
H	-5.132272	-2.218319	4.121976
H	-6.484475	-1.786969	5.204302
H	-7.176920	0.885823	3.949578
H	-6.966628	0.695016	5.709657
H	-6.080421	1.969776	4.827512
N	5.791536	0.233035	-1.547401
N	5.045789	-0.232551	-3.618014
C	6.535097	0.021016	-3.806515
C	7.052456	-0.107342	-2.333727
C	7.098156	-1.001469	-4.789642
C	6.650193	1.439805	-4.388708
C	7.426707	-1.541851	-1.924307
C	8.164085	0.861717	-1.943339
O	4.262790	-0.463824	-4.595628
O	5.813408	0.501201	-0.304654
H	7.697975	1.688931	-4.604518
H	6.081728	1.480404	-5.327149
H	6.242631	2.196747	-3.704613
H	8.173370	-0.826795	-4.936005
H	6.950504	-2.032407	-4.448148
H	6.590902	-0.888768	-5.755978
H	8.372871	0.757210	-0.871417
H	9.079960	0.625128	-2.503130

H	7.892515	1.906164	-2.134740
H	7.572777	-1.568270	-0.836293
H	6.637587	-2.260572	-2.184198
H	8.361464	-1.854786	-2.408997
C	-0.393040	0.244401	-3.531680
C	-1.663596	0.309607	-4.068637
H	0.496115	0.229758	-4.162982
C	-2.825881	0.323903	-3.241343
C	-2.735736	0.270986	-1.864342
H	-3.623061	0.284382	-1.230399
H	-1.788276	0.351119	-5.151783
H	-3.807611	0.377795	-3.714477
C	4.677108	0.022025	-2.319609

Total energy singlet BP86/def-TZVP: -1603.04562690330

Triplet BP86/def-TZVP optimized:

C	-0.243898	0.203503	-2.074985
C	-1.412608	0.210386	-1.238528
C	-0.951945	0.132759	0.090574
O	0.425525	0.085825	0.095758
C	0.865434	0.128305	-1.210264
C	-1.653165	0.093742	1.283002
C	-2.387860	0.045655	2.263768
C	-3.282402	0.012625	3.324008
C	2.221242	0.088431	-1.485113
C	3.392479	0.070421	-1.848108
N	-4.622050	0.291916	3.209037
N	-2.978076	-0.307168	4.622058
C	-5.350052	-0.060726	4.498563
C	-4.171032	-0.027831	5.529572
O	-1.833827	-0.624343	5.077237
O	-5.239915	0.614055	2.142528
C	-3.915008	1.358323	6.144352
C	-4.229182	-1.089320	6.624017
C	-5.947161	-1.460364	4.276041
C	-6.462172	0.955340	4.740965
H	-4.710740	1.621861	6.854089
H	-2.959832	1.331298	6.685279
H	-3.854560	2.141944	5.376553
H	-5.085540	-0.896796	7.285144
H	-4.316455	-2.103242	6.217076
H	-3.309685	-1.042112	7.220645
H	-6.609993	-1.423670	3.401256
H	-5.168704	-2.212171	4.088547
H	-6.537409	-1.774608	5.147551

H	-7.170388	0.918656	3.903526
H	-7.001388	0.707117	5.665886
H	-6.080735	1.979930	4.816801
N	5.823205	0.266247	-1.567254
N	5.046448	-0.259284	-3.611642
C	6.531026	-0.003848	-3.832538
C	7.074331	-0.084184	-2.365227
C	7.082657	-1.053234	-4.793668
C	6.628137	1.396855	-4.460546
C	7.471280	-1.501938	-1.920549
C	8.182055	0.907273	-2.022255
O	4.248548	-0.518617	-4.570078
O	5.863577	0.567410	-0.332597
H	7.670687	1.644110	-4.702262
H	6.043358	1.405171	-5.389694
H	6.228347	2.172736	-3.793305
H	8.154427	-0.878741	-4.963558
H	6.945588	-2.073963	-4.418781
H	6.558721	-0.971707	-5.754136
H	8.411001	0.835331	-0.951810
H	9.090479	0.664751	-2.591546
H	7.895674	1.942978	-2.238278
H	7.637764	-1.494273	-0.835203
H	6.685432	-2.236166	-2.144409
H	8.400179	-1.819619	-2.413247
C	-0.367361	0.266149	-3.483617
C	-1.639188	0.336573	-4.015943
H	0.519931	0.254136	-4.117568
C	-2.799437	0.346951	-3.184863
C	-2.705723	0.284743	-1.808865
H	-3.591176	0.295211	-1.172231
H	-1.767431	0.385263	-5.098405
H	-3.782368	0.405624	-3.654922
C	4.698629	0.026785	-2.314748

Total energy triplet BP86/def-TZVP: -1603.04499300214

Diradical X=S, ring 1

Singlet BP86/def-TZVP optimized:

C	0.581618	0.023074	-1.622929
C	-0.615121	0.008901	-0.839584
C	-0.436735	-0.017503	0.514421
S	1.354422	-0.022048	0.863743
C	1.751209	0.010470	-0.917404

C	-1.378104	-0.030096	1.541352
C	-2.238223	-0.047284	2.411872
C	-3.272358	-0.049735	3.341283
C	3.069214	0.004512	-1.368684
C	4.211690	0.001786	-1.807548
C	5.477229	-0.019190	-2.382846
N	-4.582198	0.228626	3.041633
N	-3.143021	-0.331203	4.676239
C	-5.477466	-0.080221	4.234995
C	-4.444141	-0.027300	5.411303
O	-2.070907	-0.636041	5.287978
O	-5.051707	0.528344	1.897686
C	-4.261943	1.372094	6.021974
C	-4.651938	-1.061754	6.513138
C	-6.057267	-1.480151	3.971897
C	-6.599264	0.952277	4.301983
H	-5.142616	1.655194	6.614378
H	-3.386962	1.354387	6.685287
H	-4.095245	2.136668	5.251221
H	-5.584000	-0.848988	7.055148
H	-4.694965	-2.084555	6.121771
H	-3.815843	-1.005338	7.221526
H	-6.600404	-1.461011	3.017791
H	-5.269967	-2.243704	3.905640
H	-6.758685	-1.766314	4.767128
H	-7.195762	0.895029	3.382990
H	-7.253870	0.737954	5.158151
H	-6.218289	1.975802	4.394831
N	6.653464	0.243106	-1.729819
N	5.722713	-0.303706	-3.702726
C	7.180245	-0.020865	-4.044501
C	7.842804	-0.084263	-2.626168
C	7.671851	-1.062028	-5.045725
C	7.195735	1.379384	-4.681452
C	8.301333	-1.492960	-2.213428
C	8.955423	0.929396	-2.376687
O	4.857935	-0.590064	-4.590862
H	8.209108	1.647298	-5.009233
H	6.536063	1.371614	-5.559255
H	6.836295	2.149136	-3.984938
H	8.721676	-0.865694	-5.305008
H	7.588151	-2.084020	-4.658693
H	7.067877	-0.994963	-5.959195
H	9.271028	0.866681	-1.327930
H	9.819495	0.701313	-3.016525
H	8.633008	1.958736	-2.571749
H	8.557961	-1.479494	-1.145893
H	7.513329	-2.242067	-2.370567
H	9.191326	-1.794921	-2.782003

C	-1.414844	0.031383	-2.116124
C	-0.268792	0.042399	-2.866373
H	-2.477693	0.037789	-2.344004
H	-0.052399	0.056778	-3.931557
O	6.789159	0.550607	-0.503603

Total energy singlet BP86/def-TZVP: -1848.49601923432

Triplet BP86/def-TZVP optimized:

C	0.584239	0.023609	-1.618737
C	-0.612698	0.009343	-0.835198
C	-0.433850	-0.017321	0.518585
S	1.357197	-0.021821	0.868034
C	1.753672	0.011006	-0.913151
C	-1.375364	-0.030029	1.545399
C	-2.236646	-0.047235	2.414579
C	-3.272206	-0.050371	3.342317
C	3.071792	0.004952	-1.364534
C	4.213623	0.001883	-1.804909
C	5.478320	-0.018827	-2.382437
N	-4.581460	0.228393	3.041116
N	-3.144525	-0.332909	4.677143
C	-5.478154	-0.080116	4.233469
C	-4.446010	-0.028119	5.410884
O	-2.073372	-0.639205	5.289770
O	-5.049444	0.529301	1.896809
C	-4.262914	1.370859	6.022149
C	-4.655942	-1.062564	6.512269
C	-6.058140	-1.480026	3.970693
C	-6.599211	0.953296	4.298852
H	-5.144245	1.655051	6.612936
H	-3.389115	1.351500	6.687023
H	-4.093537	2.135281	5.251838
H	-5.589077	-0.849695	7.052389
H	-4.698284	-2.085274	6.120680
H	-3.821219	-1.006279	7.222288
H	-6.598807	-1.462354	3.015195
H	-5.271045	-2.244110	3.908014
H	-6.761716	-1.764461	4.764699
H	-7.195457	0.895197	3.379719
H	-7.254262	0.741035	5.155166
H	-6.217261	1.976640	4.390037
N	6.655105	0.245610	-1.731295
N	5.722305	-0.305139	-3.702103
C	7.179355	-0.021483	-4.045812
C	7.843416	-0.083619	-2.628258

C	7.670441	-1.062822	-5.047098
C	7.193435	1.378999	-4.682284
C	8.301245	-1.491941	-2.213506
C	8.957073	0.929513	-2.381574
O	4.856813	-0.593889	-4.588785
H	8.205970	1.646668	-5.012942
H	6.531060	1.372348	-5.558039
H	6.836617	2.148394	-3.984004
H	8.720297	-0.866976	-5.306713
H	7.586435	-2.084731	-4.659871
H	7.066312	-0.995839	-5.960482
H	9.274688	0.867514	-1.333378
H	9.819727	0.700319	-3.022926
H	8.634924	1.958859	-2.576920
H	8.559435	-1.476373	-1.146351
H	7.512169	-2.240530	-2.367767
H	9.189947	-1.795973	-2.782868
C	-1.412340	0.032221	-2.111602
C	-0.266088	0.043075	-2.861888
H	-2.475223	0.039067	-2.339318
H	-0.049435	0.057510	-3.926982
O	6.792060	0.555843	-0.505970

Total energy triplet BP86/def-TZVP: -1848.49595193945

Diradical X=S, ring 2 (= no ring)

Singlet BP86/def-TZVP optimized:

C	0.596213	0.013399	-1.561667
C	-0.581726	-0.002610	-0.801413
C	-0.357999	-0.044400	0.576547
S	1.372923	-0.063605	0.933264
C	1.760385	-0.014624	-0.790466
C	-1.316443	-0.059748	1.585938
C	-2.189376	-0.077010	2.444977
C	-3.220267	-0.073084	3.376107
C	3.074315	-0.018153	-1.250146
C	4.214497	-0.014558	-1.697608
C	5.475525	-0.029605	-2.280222
H	0.629374	0.043107	-2.648927
H	-1.586576	0.016995	-1.218899
N	-4.531862	0.203680	3.081833
N	-3.084035	-0.340600	4.714077
C	-5.419404	-0.090163	4.284626
C	-4.378413	-0.020153	5.453023

O	-2.007677	-0.639497	5.322390
O	-5.007599	0.492989	1.937769
C	-4.188031	1.389506	6.037508
C	-4.582340	-1.033959	6.574346
C	-5.998748	-1.494539	4.045547
C	-6.541520	0.942279	4.344984
H	-5.063431	1.685897	6.631217
H	-3.308167	1.381238	6.694496
H	-4.025149	2.139723	5.251890
H	-5.508365	-0.806006	7.120535
H	-4.634903	-2.063230	6.201570
H	-3.739589	-0.969933	7.274106
H	-6.546768	-1.490767	3.094085
H	-5.210507	-2.257828	3.987099
H	-6.695661	-1.769701	4.848609
H	-7.145160	0.871359	3.431662
H	-7.189221	0.740112	5.209310
H	-6.160420	1.967243	4.419751
N	6.656771	0.225034	-1.632357
N	5.712744	-0.298914	-3.605288
C	7.167330	-0.010223	-3.953424
C	7.839627	-0.091767	-2.540513
C	7.652677	-1.037908	-4.971473
C	7.177517	1.398586	-4.571305
C	8.300999	-1.505535	-2.148790
C	8.954624	0.918103	-2.286577
O	4.841541	-0.575007	-4.490416
O	6.800417	0.516456	-0.402606
H	8.188299	1.671693	-4.902799
H	6.511330	1.402647	-5.444188
H	6.822807	2.158453	-3.861603
H	8.700080	-0.836714	-5.236764
H	7.573604	-2.064738	-4.596408
H	7.041235	-0.960772	-5.879193
H	9.277334	0.842700	-1.240802
H	9.813913	0.696725	-2.935116
H	8.631870	1.949942	-2.467296
H	8.565977	-1.505408	-1.083158
H	7.511647	-2.252469	-2.309273
H	9.186545	-1.800567	-2.727856

Total energy singlet BP86/def-TZVP: -1772.35891637520

Triplet BP86/def-TZVP optimized:

C	0.600512	0.016206	-1.556755
C	-0.578335	-0.001349	-0.797082

C	-0.354987	-0.045332	0.580320
S	1.375322	-0.065007	0.938221
C	1.763484	-0.013290	-0.784800
C	-1.313821	-0.060967	1.589944
C	-2.187779	-0.078953	2.447364
C	-3.220087	-0.075325	3.377513
C	3.077988	-0.017392	-1.244197
C	4.217584	-0.013373	-1.692150
C	5.477912	-0.028670	-2.277319
H	0.634594	0.047957	-2.643901
H	-1.582892	0.019310	-1.215177
N	-4.530570	0.203199	3.081674
N	-3.085370	-0.344608	4.714860
C	-5.419779	-0.090628	4.283228
C	-4.379787	-0.021319	5.452451
O	-2.010058	-0.645176	5.324226
O	-5.004387	0.494967	1.937422
C	-4.186897	1.388937	6.034718
C	-4.586099	-1.033520	6.574613
C	-5.999679	-1.494697	4.043496
C	-6.541611	0.942217	4.342193
H	-5.062613	1.688988	6.626019
H	-3.308128	1.379738	6.693173
H	-4.020560	2.136995	5.247728
H	-5.511448	-0.802921	7.120768
H	-4.640994	-2.062939	6.202538
H	-3.743081	-0.970891	7.274182
H	-6.545813	-1.490867	3.090925
H	-5.212133	-2.258821	3.987052
H	-6.698557	-1.768729	4.845290
H	-7.145279	0.869984	3.428983
H	-7.189445	0.741398	5.206743
H	-6.160359	1.967273	4.415216
N	6.659664	0.228067	-1.632199
N	5.712238	-0.300832	-3.602017
C	7.165674	-0.010813	-3.953565
C	7.840671	-0.091130	-2.542002
C	7.649846	-1.037899	-4.972731
C	7.172951	1.398022	-4.571456
C	8.300276	-1.505158	-2.149062
C	8.956908	0.918078	-2.291301
O	4.839417	-0.579661	-4.484704
O	6.805703	0.522244	-0.403379
H	8.182592	1.671886	-4.905823
H	6.504223	1.401467	-5.442418
H	6.819684	2.157578	-3.860737
H	8.696877	-0.836447	-5.239314
H	7.571167	-2.065078	-4.598451
H	7.037321	-0.960027	-5.879669

H	9.281326	0.843906	-1.245984
H	9.814982	0.695289	-2.940935
H	8.634327	1.949867	-2.472747
H	8.568113	-1.503874	-1.084137
H	7.508574	-2.250414	-2.305984
H	9.183383	-1.803388	-2.730147

Total energy triplet BP86/def-TZVP: -1772.35865451054

Diradical X=S, ring 4

Singlet BP86/def-TZVP optimized:

C	0.389828	-0.030914	-1.835919
C	-0.802255	-0.033399	-1.056344
C	-0.608280	-0.014236	0.326480
S	1.132478	0.012473	0.672067
C	1.553413	-0.005343	-1.045367
C	-1.550087	-0.013498	1.343754
C	-2.394645	-0.019824	2.232503
C	-3.366861	-0.024995	3.222887
C	2.869689	-0.002761	-1.477320
C	4.020391	0.001980	-1.902320
C	5.298428	-0.011428	-2.441065
N	-4.699394	0.229528	3.014515
N	-3.139311	-0.287231	4.550096
C	-5.502045	-0.079599	4.271886
C	-4.388986	0.005353	5.371342
O	-2.018683	-0.560733	5.087012
O	-5.253464	0.503828	1.902277
C	-4.188504	1.415020	5.952290
C	-4.500555	-1.019208	6.496582
C	-6.074182	-1.492317	4.067111
C	-6.634252	0.934545	4.406279
H	-5.030123	1.691517	6.601681
H	-3.268902	1.419602	6.552201
H	-4.089178	2.172691	5.162890
H	-5.395084	-0.814999	7.101189
H	-4.554280	-2.047150	6.120096
H	-3.616841	-0.940882	7.141975
H	-6.683472	-1.494826	3.153651
H	-5.279981	-2.242945	3.954110
H	-6.712767	-1.780045	4.913249
H	-7.290430	0.857742	3.530358
H	-7.225644	0.718203	5.306828
H	-6.265670	1.965145	4.463464

N	6.459904	0.197717	-1.741984
N	5.580519	-0.236946	-3.765775
C	7.052108	0.030934	-4.050204
C	7.669552	-0.109202	-2.616646
C	7.554447	-0.975537	-5.081890
C	7.116370	1.456972	-4.622749
C	8.094343	-1.542421	-2.255472
C	8.789504	0.873059	-2.287185
O	4.735084	-0.453943	-4.693211
O	6.561546	0.436289	-0.496400
H	8.145338	1.717810	-4.904812
H	6.486439	1.502222	-5.520807
H	6.748904	2.202622	-3.904504
H	8.615570	-0.790487	-5.300491
H	7.438430	-2.011688	-4.743774
H	6.980564	-0.855797	-6.009400
H	9.069798	0.758053	-1.232809
H	9.670136	0.659231	-2.909096
H	8.489413	1.915259	-2.445710
H	8.318142	-1.581150	-1.181061
H	7.300402	-2.270714	-2.469708
H	8.997026	-1.832677	-2.810026
C	0.130089	-0.059588	-3.245164
S	-2.236157	-0.065760	-2.070159
C	-1.207532	-0.080215	-3.510443
H	-1.690579	-0.103610	-4.484126
H	0.904184	-0.067784	-4.010312

Total energy singlet BP86/def-TZVP: -2246.84290163359

Triplet BP86/def-TZVP optimized:

C	0.350687	-0.048400	-1.891246
C	-0.840543	-0.043432	-1.108883
C	-0.643152	-0.010318	0.272536
S	1.097981	0.019195	0.613950
C	1.515043	-0.015259	-1.103620
C	-1.579905	-0.001108	1.295655
C	-2.413001	-0.000399	2.194706
C	-3.369272	-0.006981	3.201884
C	2.832424	-0.013130	-1.534811
C	3.985971	-0.008520	-1.950751
C	5.275060	-0.016371	-2.464856
N	-4.708862	0.220523	3.012712
N	-3.113940	-0.246959	4.527845
C	-5.484559	-0.088642	4.287065
C	-4.355501	0.029619	5.366786

O	-1.979236	-0.490447	5.049278
O	-5.286626	0.469757	1.906623
C	-4.173836	1.448840	5.930437
C	-4.428497	-0.985734	6.503884
C	-6.032250	-1.514516	4.107837
C	-6.633650	0.905232	4.428787
H	-5.008672	1.713966	6.593123
H	-3.243218	1.478816	6.512314
H	-4.105827	2.200587	5.131946
H	-5.320049	-0.796488	7.117694
H	-4.462763	-2.018501	6.138354
H	-3.539116	-0.880194	7.137368
H	-6.659057	-1.538814	3.206660
H	-5.225306	-2.250174	3.986665
H	-6.648032	-1.806075	4.969396
H	-7.301766	0.806307	3.564257
H	-7.206871	0.687755	5.340774
H	-6.284101	1.943233	4.469170
N	6.421278	0.166975	-1.734379
N	5.585181	-0.210806	-3.787432
C	7.064788	0.055077	-4.031248
C	7.647671	-0.130192	-2.589073
C	7.585315	-0.924907	-5.079026
C	7.151506	1.496440	-4.560343
C	8.046826	-1.577881	-2.257142
C	8.771302	0.828800	-2.208224
O	4.760008	-0.401724	-4.738584
O	6.496320	0.372093	-0.481073
H	8.188769	1.758532	-4.809084
H	6.544817	1.572005	-5.472268
H	6.770719	2.223568	-3.830085
H	8.652622	-0.740787	-5.266201
H	7.454718	-1.969481	-4.773693
H	7.035014	-0.774918	-6.016389
H	9.028253	0.680261	-1.152074
H	9.662366	0.622106	-2.817659
H	8.486748	1.878646	-2.342821
H	8.241568	-1.649141	-1.178730
H	7.250586	-2.290355	-2.512372
H	8.960526	-1.863622	-2.795763
C	0.087974	-0.090409	-3.299696
S	-2.276333	-0.085351	-2.120257
C	-1.249986	-0.113288	-3.562336
H	-1.734854	-0.145537	-4.534904
H	0.860628	-0.105510	-4.066150

Total energy triplet BP86/def-TZVP: -2246.84264493980

Diradical X=S, ring 5

Singlet BP86/def-TZVP optimized:

C	0.604348	0.003645	-1.622740
C	-0.598710	0.014951	-0.838568
C	-0.346037	0.000102	0.558400
S	1.379719	-0.017439	0.882995
C	1.780101	-0.009804	-0.826904
C	-1.289597	-0.007443	1.570751
C	-2.177049	-0.026847	2.418683
C	-3.230141	-0.034932	3.320165
C	3.087424	-0.016063	-1.280931
C	4.222000	-0.012198	-1.749577
C	5.469833	-0.026754	-2.353439
N	-4.538394	0.215649	2.984419
N	-3.132921	-0.297164	4.663150
C	-5.458339	-0.092958	4.156920
C	-4.456830	-0.005826	5.359249
O	-2.069961	-0.572364	5.306043
O	-4.983146	0.482034	1.820755
C	-4.315423	1.404327	5.956040
C	-4.676231	-1.029219	6.469339
C	-6.007441	-1.506412	3.900280
C	-6.599404	0.920838	4.180785
H	-5.215155	1.678863	6.523256
H	-3.456646	1.410641	6.640613
H	-4.143415	2.161999	5.179686
H	-5.625506	-0.825456	6.984426
H	-4.692152	-2.057586	6.090738
H	-3.859904	-0.949152	7.198224
H	-6.525799	-1.510675	2.932326
H	-5.205540	-2.256838	3.865823
H	-6.724170	-1.793265	4.681461
H	-7.169657	0.842252	3.246823
H	-7.273553	0.705479	5.021404
H	-6.238658	1.951982	4.271110
N	6.667009	0.208866	-1.726202
N	5.680016	-0.276988	-3.687807
C	7.129152	0.000279	-4.060733
C	7.828792	-0.102110	-2.661673
C	7.584775	-1.022709	-5.097782
C	7.143357	1.414165	-4.666770
C	8.292202	-1.522226	-2.296349
C	8.953280	0.900142	-2.417765
O	4.785907	-0.520407	-4.561893
O	6.836470	0.476313	-0.493792
H	8.151147	1.679877	-5.013056

H	6.462613	1.431948	-5.528197
H	6.808034	2.171516	-3.945157
H	8.628888	-0.829459	-5.381331
H	7.502541	-2.052376	-4.731230
H	6.957113	-0.930615	-5.993050
H	9.295596	0.811089	-1.379291
H	9.799186	0.683189	-3.085101
H	8.631394	1.935302	-2.580167
H	8.578281	-1.535549	-1.236222
H	7.496584	-2.264017	-2.449402
H	9.164736	-1.813795	-2.896480
C	-1.863503	0.037396	-1.480741
C	-0.716400	0.025592	-3.637238
C	0.527079	0.006526	-3.039310
H	1.443565	-0.010467	-3.630905
C	-1.908872	0.042951	-2.859869
H	-0.791100	0.027368	-4.725846
H	-2.874693	0.060793	-3.367524
H	-2.774609	0.053751	-0.880522

Total energy singlet BP86/def-TZVP: -1926.05293694008

Triplet BP86/def-TZVP optimized:

C	0.605230	0.003925	-1.622090
C	-0.598514	0.014914	-0.837496
C	-0.345370	-0.000094	0.558405
S	1.379584	-0.017428	0.882754
C	1.779855	-0.009363	-0.826317
C	-1.289324	-0.006719	1.572087
C	-2.176647	-0.026686	2.419328
C	-3.231179	-0.035230	3.320965
C	3.088496	-0.016277	-1.280233
C	4.222471	-0.012215	-1.748944
C	5.471178	-0.026798	-2.353822
N	-4.538388	0.216290	2.984568
N	-3.133565	-0.297712	4.663095
C	-5.458831	-0.092733	4.156811
C	-4.457516	-0.006247	5.359280
O	-2.071177	-0.574405	5.306096
O	-4.982603	0.483737	1.820910
C	-4.315604	1.403834	5.956386
C	-4.677060	-1.029671	6.469238
C	-6.007920	-1.506170	3.899817
C	-6.599676	0.921164	4.180522
H	-5.215416	1.678622	6.523358
H	-3.457046	1.409680	6.641206

H	-4.143114	2.161665	5.180299
H	-5.626408	-0.825571	6.984047
H	-4.692987	-2.058076	6.090726
H	-3.860869	-0.949830	7.198332
H	-6.525966	-1.510569	2.931727
H	-5.206030	-2.256635	3.865807
H	-6.724938	-1.793030	4.680758
H	-7.169630	0.842784	3.246369
H	-7.274032	0.705766	5.020973
H	-6.238623	1.952183	4.270986
N	6.667384	0.209619	-1.726792
N	5.680250	-0.277939	-3.687553
C	7.129251	-0.000137	-4.061182
C	7.829196	-0.101719	-2.662306
C	7.584745	-1.023120	-5.098116
C	7.143080	1.413719	-4.667342
C	8.292495	-1.521758	-2.296277
C	8.953635	0.900563	-2.418768
O	4.785849	-0.522859	-4.560953
O	6.837358	0.478982	-0.494974
H	8.150782	1.679381	-5.013997
H	6.462076	1.431536	-5.528527
H	6.808184	2.171126	-3.945588
H	8.628742	-0.829769	-5.382053
H	7.502640	-2.052664	-4.731209
H	6.956697	-0.931197	-5.993119
H	9.296147	0.811910	-1.380312
H	9.799302	0.683148	-3.086253
H	8.631812	1.935706	-2.581341
H	8.578841	-1.534480	-1.236251
H	7.496801	-2.263611	-2.448767
H	9.164787	-1.813811	-2.896538
C	-1.863532	0.037447	-1.480056
C	-0.715740	0.025702	-3.636500
C	0.527627	0.006710	-3.039019
H	1.443896	-0.010531	-3.630910
C	-1.908574	0.043150	-2.858892
H	-0.790815	0.027539	-4.725045
H	-2.874236	0.061011	-3.366782
H	-2.774874	0.053951	-0.880226

Total energy **triplet** BP86/def-TZVP: -1926.05247599246

Junction X=O, ring 1

C	-3.10999175	0.00000000	0.71988886

C	-3.10990979	0.00000000	-0.71991153
C	-1.81631575	0.00000000	-1.13832288
C	-1.81635665	0.00000000	1.13833016
O	-0.97219542	0.00000000	-0.00003892
C	-1.17805491	0.00000000	2.38468212
C	-0.61932539	0.00000000	3.47263805
C	-1.17795299	0.00000000	-2.38462468
C	-0.61874156	0.00000000	-3.47234066
C	-4.61131651	0.00000000	0.68539091
C	-4.61114428	0.00000000	-0.68565285
H	-5.38681010	0.00000000	-1.44666208
H	-5.38735723	0.00000000	1.44609112
S	0.00006889	0.00000000	5.03458222
S	-0.00000000	0.00000000	-5.03458261
Au	-1.44000000	-0.83137561	9.22347988
Au	1.44000000	-0.83137561	9.22347988
Au	0.00000000	1.66277439	9.22347988
Au	0.00000000	-1.66276561	6.87196988
Au	1.44000000	0.83138439	6.87196988
Au	-1.44000000	0.83138439	6.87196988
Au	-2.88000000	-1.66276561	6.87196988
Au	2.88000000	-1.66276561	6.87196988
Au	0.00000000	3.32554439	6.87196988
Au	-1.44000000	-0.83137561	-9.22347988
Au	1.44000000	-0.83137561	-9.22347988
Au	0.00000000	1.66277439	-9.22347988
Au	0.00000000	-1.66276561	-6.87196988
Au	1.44000000	0.83138439	-6.87196988
Au	-1.44000000	0.83138439	-6.87196988
Au	-2.88000000	-1.66276561	-6.87196988
Au	2.88000000	-1.66276561	-6.87196988
Au	0.00000000	3.32554439	-6.87196988

Total energy BP86/LANL2DZ: -2917.66727860

Junction X=O, ring 2 (= no ring)

C	-3.04582225	-0.00000000	0.70776264
C	-3.04475203	-0.00000000	-0.70925831
C	-1.72187090	-0.00000000	-1.10956323
C	-1.72352402	-0.00000000	1.11008436
O	-0.89911540	-0.00000000	0.00076379
C	-1.11505626	-0.00000000	2.37172815
C	-0.58346605	-0.00000000	3.47341571
C	-1.11216101	-0.00000000	-2.37050747
C	-0.58278849	-0.00000000	-3.47320678

H	-3.90627708	-0.00000000	1.36790466
H	-3.90412223	-0.00000000	-1.37079742
S	-0.00006866	-0.00000000	5.05117793
S	0.00000000	-0.00000000	-5.05117750
Au	-1.44000000	-0.83137561	9.24007560
Au	1.44000000	-0.83137561	9.24007560
Au	0.00000000	1.66277439	9.24007560
Au	0.00000000	-1.66276561	6.88856560
Au	1.44000000	0.83138439	6.88856560
Au	-1.44000000	0.83138439	6.88856560
Au	-2.88000000	-1.66276561	6.88856560
Au	2.88000000	-1.66276561	6.88856560
Au	0.00000000	3.32554439	6.88856560
Au	-1.44000000	-0.83137561	-9.24007560
Au	1.44000000	-0.83137561	-9.24007560
Au	0.00000000	1.66277439	-9.24007560
Au	0.00000000	-1.66276561	-6.88856560
Au	1.44000000	0.83138439	-6.88856560
Au	-1.44000000	0.83138439	-6.88856560
Au	-2.88000000	-1.66276561	-6.88856560
Au	2.88000000	-1.66276561	-6.88856560
Au	0.00000000	3.32554439	-6.88856560

Total energy BP86/LANL2DZ: -2841.58058904

Junction X=O, ring 3

C	-0.86106989	-2.99667475	-0.68725825
C	-0.91825119	-3.01706954	0.72245845
C	-0.56104270	-1.73556094	1.14130001
C	-0.48087055	-1.74256884	-1.13578069
O	-0.29788531	-0.96830977	0.00988929
C	-0.27286351	-1.17526552	-2.38537907
C	-0.06852100	-0.70227201	-3.49955991
C	-0.42565990	-1.13931181	2.38892907
C	-0.33604795	-0.62946365	3.50251293
C	-1.31795711	-4.35401689	1.06937195
C	-1.46310609	-5.00550338	-0.11934187
H	-1.47774362	-4.78253061	2.05268256
O	-1.19050786	-4.20381887	-1.22494135
H	-1.74854681	-6.02293921	-0.36354919
S	-0.00000121	0.00000000	5.01516330
S	0.00000000	0.00000000	-5.01516342
Au	-1.44000000	-0.83137561	9.20406097
Au	1.44000000	-0.83137561	9.20406097
Au	0.00000000	1.66277439	9.20406097

Au	0.00000000	-1.66276561	6.85255097
Au	1.44000000	0.83138439	6.85255097
Au	-1.44000000	0.83138439	6.85255097
Au	-2.88000000	-1.66276561	6.85255097
Au	2.88000000	-1.66276561	6.85255097
Au	0.00000000	3.32554439	6.85255097
Au	-1.44000000	-0.83137561	-9.20406097
Au	1.44000000	-0.83137561	-9.20406097
Au	0.00000000	1.66277439	-9.20406097
Au	0.00000000	-1.66276561	-6.85255097
Au	1.44000000	0.83138439	-6.85255097
Au	-1.44000000	0.83138439	-6.85255097
Au	-2.88000000	-1.66276561	-6.85255097
Au	2.88000000	-1.66276561	-6.85255097
Au	0.00000000	3.32554439	-6.85255097

Total energy BP86/LANL2DZ: -2992.96569557

Junction X=O, ring 4

C	0.68280434	-3.04468336	0.70523241
C	0.68573267	-3.05842683	-0.72117162
C	0.31576288	-1.77393281	-1.12921200
C	0.31662984	-1.77240114	1.12914207
O	0.09290722	-0.99939504	-0.00241879
C	0.15655308	-1.19275066	2.38192936
C	0.00065012	-0.71362108	3.50144663
C	0.15471687	-1.19194836	-2.38092532
C	-0.00142865	-0.71315798	-3.50103965
C	1.05328619	-4.33368523	-1.25518014
C	1.31123841	-5.22845787	-0.25638157
H	1.12243276	-4.57246524	-2.31405504
S	1.12698193	-4.58288189	1.36563027
H	1.61117250	-6.26789696	-0.36398811
S	-0.00014302	0.00000000	5.01387251
S	0.00000000	0.00000000	-5.01387215
Au	-1.44000000	-0.83137561	9.20277017
Au	1.44000000	-0.83137561	9.20277017
Au	0.00000000	1.66277439	9.20277017
Au	0.00000000	-1.66276561	6.85126017
Au	1.44000000	0.83138439	6.85126017
Au	-1.44000000	0.83138439	6.85126017
Au	-2.88000000	-1.66276561	6.85126017
Au	2.88000000	-1.66276561	6.85126017
Au	0.00000000	3.32554439	6.85126017
Au	-1.44000000	-0.83137561	-9.20277017

Au	1.44000000	-0.83137561	-9.20277017
Au	0.00000000	1.66277439	-9.20277017
Au	0.00000000	-1.66276561	-6.85126017
Au	1.44000000	0.83138439	-6.85126017
Au	-1.44000000	0.83138439	-6.85126017
Au	-2.88000000	-1.66276561	-6.85126017
Au	2.88000000	-1.66276561	-6.85126017
Au	0.00000000	3.32554439	-6.85126017

Total energy BP86/LANL2DZ: -2927.89325252

Junction X=O, ring 5

C	-3.10879115	-0.26051759	0.72046793
C	-3.11119813	-0.25787778	-0.71725387
C	-1.76592367	-0.22264357	-1.12300298
C	-1.76228006	-0.22554507	1.12201485
O	-0.96462695	-0.20303834	-0.00178788
C	-1.16039455	-0.20618976	2.37339560
C	-0.66727242	-0.21495956	3.49871301
C	-1.16687879	-0.20325700	-2.37585250
C	-0.67176930	-0.21219144	-3.50033007
C	-4.33363678	-0.28771616	-1.43143138
C	-4.32839031	-0.29407272	1.43908210
C	-5.50380686	-0.32405363	0.71973265
H	-4.32690202	-0.29558109	2.52943931
C	-5.50637614	-0.32063043	-0.70791502
H	-4.33617809	-0.28451767	-2.52171206
H	-6.45842283	-0.35076230	1.24692636
H	-6.46290117	-0.34418402	-1.23158834
S	0.00000033	0.00000000	5.01695393
S	-0.00000000	0.00000000	-5.01695395
Au	-1.44000000	-0.83137561	9.20585159
Au	1.44000000	-0.83137561	9.20585159
Au	0.00000000	1.66277439	9.20585159
Au	0.00000000	-1.66276561	6.85434159
Au	1.44000000	0.83138439	6.85434159
Au	-1.44000000	0.83138439	6.85434159
Au	-2.88000000	-1.66276561	6.85434159
Au	2.88000000	-1.66276561	6.85434159
Au	0.00000000	3.32554439	6.85434159
Au	-1.44000000	-0.83137561	-9.20585159
Au	1.44000000	-0.83137561	-9.20585159
Au	0.00000000	1.66277439	-9.20585159
Au	0.00000000	-1.66276561	-6.85434159
Au	1.44000000	0.83138439	-6.85434159

Au	-1.44000000	0.83138439	-6.85434159
Au	-2.88000000	-1.66276561	-6.85434159
Au	2.88000000	-1.66276561	-6.85434159
Au	0.00000000	3.32554439	-6.85434159

Total energy BP86/LANL2DZ: -2995.19697600

Junction X=S, ring 1

C	-2.39304234	-0.00000000	0.71630479
C	-2.39114227	-0.00000000	-0.71862147
C	-1.15977195	-0.00000000	-1.30353112
C	-1.16308112	-0.00000000	1.30421710
S	0.08849961	0.00000000	0.00186518
C	-0.75954049	-0.00000000	2.64410882
C	-0.36529297	-0.00000000	3.80336527
C	-0.75415714	-0.00000000	-2.64284408
C	-0.35961837	-0.00000000	-3.80206378
C	-3.89656668	-0.00000000	0.68195007
C	-3.89467499	-0.00000000	-0.68855924
H	-4.67105858	-0.00000000	-1.44914448
H	-4.67528691	-0.00000000	1.44009258
S	0.00000295	0.00000000	5.44265602
S	0.00000000	0.00000000	-5.44265604
Au	-1.44000000	-0.83137561	9.63155369
Au	1.44000000	-0.83137561	9.63155369
Au	0.00000000	1.66277439	9.63155369
Au	0.00000000	-1.66276561	7.28004369
Au	1.44000000	0.83138439	7.28004369
Au	-1.44000000	0.83138439	7.28004369
Au	-2.88000000	-1.66276561	7.28004369
Au	2.88000000	-1.66276561	7.28004369
Au	0.00000000	3.32554439	7.28004369
Au	-1.44000000	-0.83137561	-9.63155369
Au	1.44000000	-0.83137561	-9.63155369
Au	0.00000000	1.66277439	-9.63155369
Au	0.00000000	-1.66276561	-7.28004369
Au	1.44000000	0.83138439	-7.28004369
Au	-1.44000000	0.83138439	-7.28004369
Au	-2.88000000	-1.66276561	-7.28004369
Au	2.88000000	-1.66276561	-7.28004369
Au	0.00000000	3.32554439	-7.28004369

Total energy BP86/LANL2DZ: -2852.60003139

Junction X=S, ring 2 (= no ring)

C	-2.30291385	0.00000000	-0.70103219
C	-2.29851690	0.00000000	0.70733536
C	-1.02109469	0.00000000	1.25898760
C	-1.02879083	0.00000000	-1.26038505
S	0.18903791	-0.00000000	-0.00422320
C	-0.65987764	0.00000000	-2.61141567
C	-0.30733599	0.00000000	-3.78414969
C	-0.64826616	0.00000000	2.60896869
C	-0.30038573	0.00000000	3.78304337
H	-3.20377762	0.00000000	-1.31102254
H	-3.19498815	0.00000000	1.32375746
S	-0.00002084	0.00000000	5.43710124
S	0.00000000	0.00000000	-5.43710136
Au	-1.44000000	-0.83137561	9.62599890
Au	1.44000000	-0.83137561	9.62599890
Au	0.00000000	1.66277439	9.62599890
Au	0.00000000	-1.66276561	7.27448890
Au	1.44000000	0.83138439	7.27448890
Au	-1.44000000	0.83138439	7.27448890
Au	-2.88000000	-1.66276561	7.27448890
Au	2.88000000	-1.66276561	7.27448890
Au	0.00000000	3.32554439	7.27448890
Au	-1.44000000	-0.83137561	-9.62599890
Au	1.44000000	-0.83137561	-9.62599890
Au	0.00000000	1.66277439	-9.62599890
Au	0.00000000	-1.66276561	-7.27448890
Au	1.44000000	0.83138439	-7.27448890
Au	-1.44000000	0.83138439	-7.27448890
Au	-2.88000000	-1.66276561	-7.27448890
Au	2.88000000	-1.66276561	-7.27448890
Au	0.00000000	3.32554439	-7.27448890

Total energy BP86/LANL2DZ: -2776.49857868

Junction X=S, ring 3

C	-2.29214622	0.02616584	0.69404004
C	-2.33386849	0.02535255	-0.72131751
C	-1.05846076	0.01236037	-1.29229445
C	-1.03994132	0.01405426	1.28844492
S	0.14686668	0.00079820	-0.01199640
C	-0.66559421	0.01048077	2.63290492
C	-0.30997187	0.00686114	3.80487660
C	-0.67637241	0.00819366	-2.63445517

C	-0.31929613	0.00419438	-3.80706817
C	-3.73224876	0.03865146	-1.06402241
C	-4.40070444	0.04602435	0.12199303
H	-4.18347648	0.04215380	-2.05015461
O	-3.55534446	0.03876722	1.22335893
H	-5.45761278	0.05631215	0.36508863
S	0.00000056	0.00000000	5.45782851
S	0.00000000	-0.00000000	-5.45782852
Au	-1.44000000	-0.83137561	9.64672617
Au	1.44000000	-0.83137561	9.64672617
Au	0.00000000	1.66277439	9.64672617
Au	0.00000000	-1.66276561	7.29521617
Au	1.44000000	0.83138439	7.29521617
Au	-1.44000000	0.83138439	7.29521617
Au	-2.88000000	-1.66276561	7.29521617
Au	2.88000000	-1.66276561	7.29521617
Au	0.00000000	3.32554439	7.29521617
Au	-1.44000000	-0.83137561	-9.64672617
Au	1.44000000	-0.83137561	-9.64672617
Au	0.00000000	1.66277439	-9.64672617
Au	0.00000000	-1.66276561	-7.29521617
Au	1.44000000	0.83138439	-7.29521617
Au	-1.44000000	0.83138439	-7.29521617
Au	-2.88000000	-1.66276561	-7.29521617
Au	2.88000000	-1.66276561	-7.29521617
Au	0.00000000	3.32554439	-7.29521617

Total energy BP86/LANL2DZ: -2927.89292552

Junction X=S, ring 4

C	0.12143063	2.30656236	0.70765207
C	0.12134907	2.32839271	-0.72133297
C	0.05540073	1.04296978	-1.27817665
C	0.05695736	1.03737836	1.27701399
S	-0.00546339	-0.15521304	-0.00652081
C	0.03813850	0.65955246	2.62114786
C	0.02042490	0.30914397	3.79508438
C	0.03582891	0.66605020	-2.62225468
C	0.01735757	0.31317530	-3.79603704
C	0.18888993	3.66266852	-1.24169584
C	0.23694422	4.59292571	-0.24528961
H	0.20064722	3.91094586	-2.30084551
S	0.20377689	3.91603635	1.37006869
H	0.29169421	5.67323978	-0.35222251
S	0.00146213	0.00000000	5.44771531

S	-0.00000000	0.00000000	-5.44771576
Au	-1.44000000	-0.83137561	9.63661297
Au	1.44000000	-0.83137561	9.63661297
Au	0.00000000	1.66277439	9.63661297
Au	0.00000000	-1.66276561	7.28510297
Au	1.44000000	0.83138439	7.28510297
Au	-1.44000000	0.83138439	7.28510297
Au	-2.88000000	-1.66276561	7.28510297
Au	2.88000000	-1.66276561	7.28510297
Au	0.00000000	3.32554439	7.28510297
Au	-1.44000000	-0.83137561	-9.63661297
Au	1.44000000	-0.83137561	-9.63661297
Au	0.00000000	1.66277439	-9.63661297
Au	0.00000000	-1.66276561	-7.28510297
Au	1.44000000	0.83138439	-7.28510297
Au	-1.44000000	0.83138439	-7.28510297
Au	-2.88000000	-1.66276561	-7.28510297
Au	2.88000000	-1.66276561	-7.28510297
Au	0.00000000	3.32554439	-7.28510297

Total energy BP86/LANL2DZ: -2862.81580858

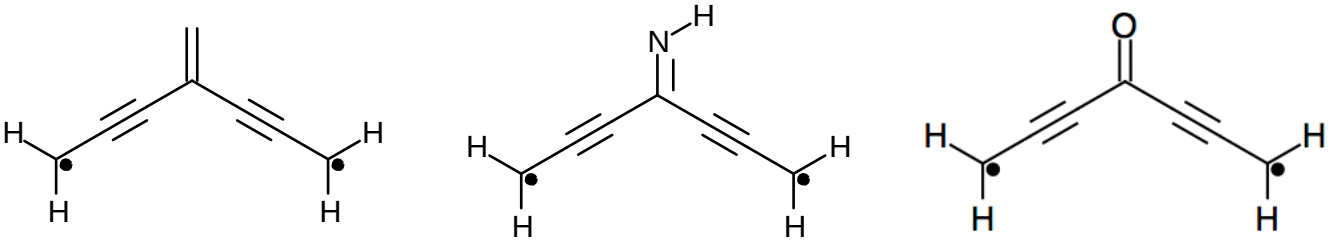
Junction X=S, ring 5

C	-2.45615160	-0.19962564	0.71910364
C	-2.45738376	-0.19834217	-0.71810548
C	-1.15094454	-0.18253118	-1.26853075
C	-1.14877991	-0.18285889	1.26732159
S	0.03284625	-0.16610419	-0.00164593
C	-0.77361830	-0.17609354	2.60947986
C	-0.43853691	-0.19501735	3.79130450
C	-0.77767956	-0.17865471	-2.61119289
C	-0.44598004	-0.19991887	-3.79392398
C	-3.68846640	-0.21291294	-1.42258345
C	-3.68594738	-0.21637056	1.42561908
C	-4.86641815	-0.23204294	0.71432688
H	-3.67928984	-0.21666243	2.51617758
C	-4.86768752	-0.22999201	-0.70939751
H	-3.68336707	-0.21055927	-2.51312888
H	-5.81861089	-0.24625760	1.24653603
H	-5.82081127	-0.24172756	-1.23978761
S	0.00000961	-0.00000000	5.39571955
S	0.00000000	-0.00000000	-5.39572001
Au	-1.44000000	-0.83137561	9.58461721
Au	1.44000000	-0.83137561	9.58461721
Au	0.00000000	1.66277439	9.58461721

Au	0.00000000	-1.66276561	7.23310721
Au	1.44000000	0.83138439	7.23310721
Au	-1.44000000	0.83138439	7.23310721
Au	-2.88000000	-1.66276561	7.23310721
Au	2.88000000	-1.66276561	7.23310721
Au	0.00000000	3.32554439	7.23310721
Au	-1.44000000	-0.83137561	-9.58461721
Au	1.44000000	-0.83137561	-9.58461721
Au	0.00000000	1.66277439	-9.58461721
Au	0.00000000	-1.66276561	-7.23310721
Au	1.44000000	0.83138439	-7.23310721
Au	-1.44000000	0.83138439	-7.23310721
Au	-2.88000000	-1.66276561	-7.23310721
Au	2.88000000	-1.66276561	-7.23310721
Au	0.00000000	3.32554439	-7.23310721

Total energy BP86/LANL2DZ: -2930.11505987

2.3 Cross-conjugated systems



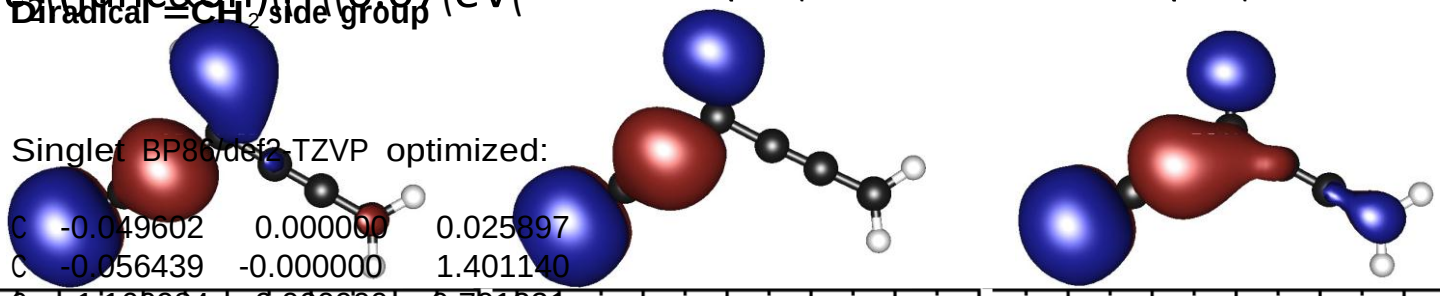
E_T,E_{BS}(((=(((,17.0(kJ/mol((,6.0(kJ/mol((12.5(kJ/mol(

ε_1,ε_2(((((=(((((9.2(kJ/mol(44.5(kJ/mol(((70.0(kJ/mol(

ε_1,ε_2((junc&on)((=((6.07(eV(6.48(eV(6.92(eV(

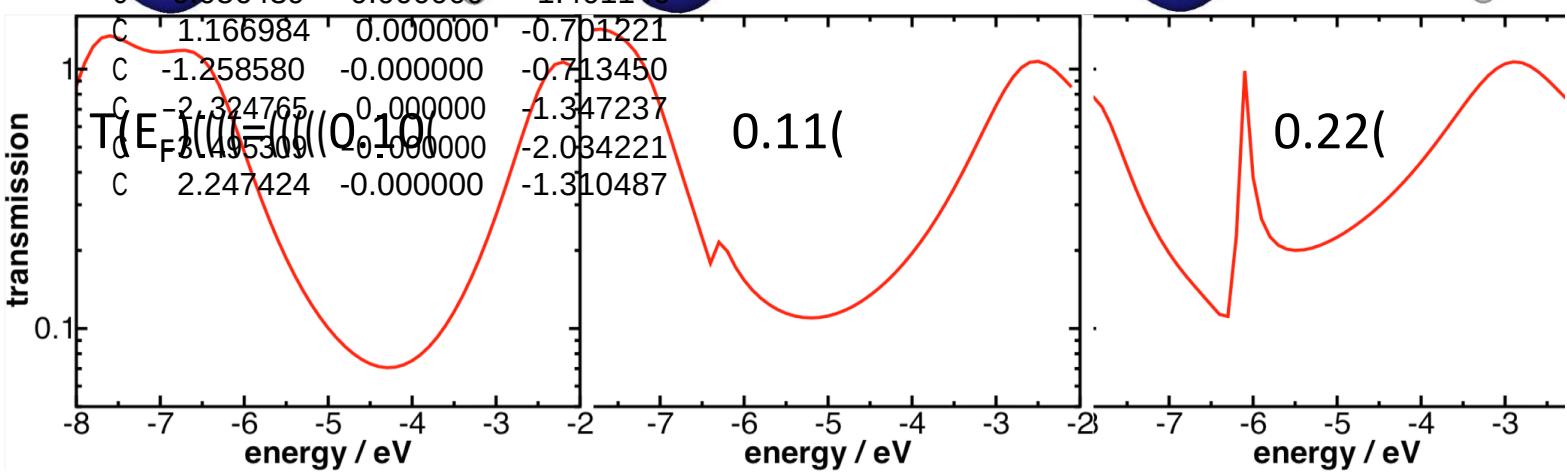
Figure 3: Lewis structures of cross-conjugated diradicals. In the junctions, the CH_2 radical groups are replaced by Si-Au units (with the structures constructed as described in the methodology section).

Diradical $=CH_2$ side group



Singlet BP86/def2-TZVP optimized:

C	-0.049602	0.000000	0.025897
C	-0.056439	-0.000000	1.401140
C	1.166984	0.000000	-0.701221
C	-1.258580	-0.000000	-0.713450
C	-2.324765	0.000000	-1.347237
C	-3.495309	-0.000000	-2.034221
C	2.247424	-0.000000	-1.310487



H	-3.508882	0.000000	-3.124659
C	3.425176	-0.000000	-1.985175
H	4.378177	0.000000	-1.454929
H	3.448583	0.000000	-3.075606
H	0.878408	0.000000	1.958117
H	-0.996811	-0.000000	1.948874

Total energy singlet BP86/def2-TZVP: -308.35933608942

Triplet BP86/def2-TZVP optimized:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.329974
C	1.255713	0.000000	-0.724986
C	-1.255713	0.000000	-0.724986
C	-2.285397	0.000000	-1.319474
C	-3.541109	0.000000	-2.044461
C	2.285397	0.000000	-1.319474
H	-4.484193	0.000000	-1.499971
H	-3.541109	0.000000	-3.133439
C	3.338418	0.000000	-1.903174
H	4.271855	0.000000	-1.342308
H	3.357424	0.000000	-2.991987
H	0.943084	0.000000	1.874464
H	-0.943084	0.000000	1.874464

Total energy triplet BP86/def2-TZVP: -308.36581585968

Singlet B3LYP/def2-TZVP optimized:

C	-0.048077	-0.000243	0.032395
C	-0.059264	-0.000008	1.391436
C	1.171644	-0.000304	-0.692872
C	-1.256439	-0.000311	-0.711554
C	-2.310019	0.000030	-1.341901
C	-3.477556	0.000073	-2.032149
C	2.234219	0.000168	-1.307828
H	-4.428830	0.000131	-1.515608
H	-3.486408	0.000040	-3.114529
C	3.408431	0.000085	-1.986785
H	4.355313	0.000121	-1.462294
H	3.426325	-0.000048	-3.069072
H	0.865298	0.000126	1.950742
H	-0.993351	0.000139	1.934661

Total energy singlet B3LYP/def2-TZVP: -308.15618012975

Triplet B3LYP/def2-TZVP optimized:

C	-0.047866	0.000009	0.000950
C	-0.059095	-0.000014	1.386165
C	1.163631	-0.000102	-0.707454
C	-1.248678	0.000060	-0.725511
C	-2.315335	0.000109	-1.344446
C	-3.481520	-0.000007	-2.019914
C	2.238937	0.000137	-1.311273
H	-4.429391	-0.000031	-1.496247
H	-3.501019	-0.000085	-3.102419
C	3.412138	0.000020	-1.974559
H	4.355105	-0.000047	-1.442393
H	3.441978	-0.000014	-3.056923
H	0.867117	-0.000081	1.942277
H	-0.994716	0.000046	1.926390

Total energy triplet B3LYP/def2-TZVP: -308.16394638069

Diradical =NH side group

Singlet BP86/def2-TZVP optimized:

C	-0.050819	0.000856	0.104124
N	-0.097940	0.000536	1.415546
C	1.146597	-0.000273	-0.668515
C	-1.256831	0.002028	-0.652126
C	-2.304991	-0.001608	-1.315105
C	-3.456174	-0.000644	-2.029752
C	2.221321	0.002005	-1.291150
H	-4.425806	-0.002372	-1.529777
H	-3.443243	0.002252	-3.120563
C	3.391715	-0.000033	-1.975347
H	4.349682	-0.001980	-1.453232
H	3.405936	-0.000290	-3.066259
H	0.864924	-0.000477	1.782336

Total energy singlet BP86/def2-TZVP: -324.41523202878

Triplet BP86/def2-TZVP optimized:

C	-0.052590	-0.000000	0.054138
N	-0.094823	0.000000	1.382965
C	1.154883	-0.000000	-0.683948
C	-1.268272	0.000000	-0.668116
C	-2.326319	0.000000	-1.318427
C	-3.488088	0.000000	-2.011308
C	2.240127	-0.000000	-1.291536
H	-4.449049	0.000000	-1.494783
H	-3.494540	-0.000000	-3.102089
C	3.421473	-0.000000	-1.951442
H	4.368943	-0.000000	-1.410427
H	3.457979	0.000000	-3.041821
H	0.874645	0.000000	1.736971

Total energy triplet BP86/def2-TZVP: -324.41770742709

Singlet B3LYP/def2-TZVP optimized:

C	-0.049650	-0.000214	0.089500
N	-0.097892	0.000140	1.382562
C	1.156885	-0.000560	-0.674038
C	-1.257886	-0.000390	-0.666427
C	-2.300733	0.000293	-1.313859
C	-3.456996	0.000062	-2.019320
C	2.221913	0.000356	-1.286370
H	-4.414708	0.000020	-1.514347
H	-3.451151	0.000014	-3.101937
C	3.394127	0.000059	-1.966786
H	4.342160	-0.000011	-1.443959
H	3.409782	0.000018	-3.049332
H	0.848518	0.000214	1.764490

Total energy singlet B3LYP/def2-TZVP: -324.20334821495

Triplet B3LYP/def2-TZVP optimized:

C	-0.051294	0.000010	0.046272
N	-0.092910	-0.000052	1.363281
C	1.156294	0.000088	-0.687239
C	-1.264402	-0.000018	-0.674802
C	-2.315851	0.000011	-1.315067
C	-3.474816	-0.000001	-2.005258

C	2.231858	0.000031	-1.288938
H	-4.427814	-0.000019	-1.491189
H	-3.480885	0.000014	-3.088015
C	3.409526	-0.000016	-1.947690
H	4.349439	0.000008	-1.410010
H	3.443654	-0.000055	-3.030016
H	0.861571	0.000000	1.728852

Total energy triplet B3LYP/def2-TZVP: -324.20814125408

Diradical =O side group

Singlet BP86/def2-TZVP optimized:

C	-0.064215	0.000000	0.080608
O	-0.066366	0.000000	1.323055
C	1.137177	-0.000000	-0.701456
C	-1.259660	0.000000	-0.709562
C	-2.329580	-0.000000	-1.344483
C	-3.497417	-0.000000	-2.023162
C	2.229009	-0.000000	-1.298288
H	-4.452322	0.000000	-1.494423
H	-3.519169	-0.000000	-3.114187
C	3.411675	-0.000000	-1.950648
H	4.354498	0.000000	-1.400689
H	3.457656	-0.000000	-3.041050

Total energy singlet BP86/def2-TZVP: -344.30696052293

Triplet BP86/def2-TZVP optimized:

C	-0.063769	0.000000	0.061035
O	-0.074582	0.000003	1.309397
C	1.162137	-0.000003	-0.679904
C	-1.276351	0.000001	-0.701396
C	-2.344150	0.000000	-1.333180
C	-3.512747	-0.000001	-2.022146
C	2.242203	-0.000002	-1.290618
H	-4.471494	0.000010	-1.501425
H	-3.521883	-0.000014	-3.113115
C	3.426609	0.000001	-1.952212
H	4.372325	-0.000013	-1.408110
H	3.462988	0.000017	-3.042611

Total energy triplet BP86/def2-TZVP: -344.30236633099

Singlet B3LYP/def2-TZVP optimized:

C	-0.063911	-0.000003	0.071292
O	-0.075447	0.000037	1.297850
C	1.148586	-0.000082	-0.694180
C	-1.261598	0.000030	-0.717073
C	-2.323633	0.000012	-1.338471
C	-3.490318	-0.000006	-2.019067
C	2.223236	-0.000038	-1.293594
H	-4.437995	0.000027	-1.494776
H	-3.507030	-0.000041	-3.101911
C	3.404318	0.000009	-1.948984
H	4.340403	-0.000018	-1.404198
H	3.444675	0.000074	-3.031174

Total energy singlet B3LYP/def2-TZVP: -344.09055899618

Triplet B3LYP/def2-TZVP optimized:

C	-0.063675	-0.000004	0.049898
O	-0.074729	0.000016	1.285816
C	1.162632	0.000065	-0.684996
C	-1.276307	-0.000080	-0.707274
C	-2.334476	-0.000016	-1.332254
C	-3.501588	0.000016	-2.017368
C	2.233306	0.000007	-1.288588
H	-4.451315	-0.000008	-1.497308
H	-3.512355	0.000034	-3.100096
C	3.415467	-0.000015	-1.947286
H	4.352920	0.000006	-1.405349
H	3.451405	-0.000020	-3.029479

Total energy triplet B3LYP/def2-TZVP: -344.08912224923

Junction $=CH_2$ side group

C	0.00000000	3.59185400	5.54013800
H	0.00000000	4.14591300	6.47646100
C	0.00000000	1.46975700	6.74612200

C	0.00000000	1.46965700	4.33422100
C	0.00000000	0.78327100	3.32321200
C	0.00000000	0.78327600	7.75705900
H	0.00000000	4.14597700	4.60385300
C	0.00000000	2.23120600	5.54014200
S	0.00000000	0.00008400	9.24293900
S	0.00000000	0.00000000	1.83735200
Au	-1.44000000	-0.83137561	-2.35151000
Au	1.44000000	-0.83137561	-2.35151000
Au	0.00000000	1.66277439	-2.35151000
Au	0.00000000	-1.66276561	0.00000000
Au	1.44000000	0.83138439	0.00000000
Au	-1.44000000	0.83138439	0.00000000
Au	-2.88000000	-1.66276561	0.00000000
Au	2.88000000	-1.66276561	0.00000000
Au	0.00000000	3.32554439	0.00000000
AU	-1.43997200	-0.83135900	13.43157700
AU	1.43997200	-0.83135900	13.43157700
AU	0.00000000	1.66274200	13.43157700
AU	0.00000000	-1.66273300	11.08011300
AU	1.43997200	0.83136800	11.08011300
AU	-1.43997200	0.83136800	11.08011300
AU	-2.87994400	-1.66273300	11.08011300
AU	2.87994400	-1.66273300	11.08011300
AU	0.00000000	3.32548000	11.08011300

Total energy BP86/LANL2DZ: -2690.15203130

Junction =NH side group

C	2.18537	0.	-0.00106
N	3.48617	0.	-0.02786
C	1.44004	0.	-1.22148
C	1.39545	0.	1.19262
C	0.73637	0.	2.22436
C	0.75656	0.	-2.235
H	3.84578	0.	0.93721
S	0.00014	0.	3.72909
S	0.	0.	-3.72909
Au	-1.44	-0.83138	7.91798
Au	1.44	-0.83138	7.91798
Au	0.	1.66277	7.91798
Au	0.	-1.66277	5.56647
Au	1.44	0.83138	5.56647
Au	-1.44	0.83138	5.56647
Au	-2.88	-1.66277	5.56647
Au	2.88	-1.66277	5.56647
Au	0.	3.32554	5.56647

Au	-1.44	-0.83138	-7.91798
Au	1.44	-0.83138	-7.91798
Au	0.	1.66277	-7.91798
Au	0.	-1.66277	-5.56647
Au	1.44	0.83138	-5.56647
Au	-1.44	0.83138	-5.56647
Au	-2.88	-1.66277	-5.56647
Au	2.88	-1.66277	-5.56647
Au	0.	3.32554	-5.56647

Total energy BP86/LANL2DZ: -2706.18811264

Junction =O side group

C	0.00000000	-2.10456900	5.61577800
O	0.00000000	-3.33998000	5.61572100
C	0.00000000	-1.33251400	4.40208800
C	0.00000000	-1.33259000	6.82951600
C	0.00000000	-0.69315500	7.87473600
S	0.00000000	0.00001900	9.39419200
C	0.00000000	-0.69318500	3.35680300
S	0.00000000	0.00000000	1.83735200
AU	-1.43999961	-0.83137546	13.58308910
AU	1.43999961	-0.83137546	13.58308910
AU	0.00000000	1.66277421	13.58308910
AU	0.00000000	-1.66276522	11.23157966
AU	1.43999961	0.83138446	11.23157966
AU	-1.43999961	0.83138446	11.23157966
AU	-2.87999975	-1.66276522	11.23157966
AU	2.87999975	-1.66276522	11.23157966
AU	0.00000000	3.32554419	11.23157966
Au	-1.44000000	-0.83137561	-2.35151000
Au	1.44000000	-0.83137561	-2.35151000
Au	0.00000000	1.66277439	-2.35151000
Au	0.00000000	-1.66276561	0.00000000
Au	1.44000000	0.83138439	0.00000000
Au	-1.44000000	0.83138439	0.00000000
Au	-2.88000000	-1.66276561	0.00000000
Au	2.88000000	-1.66276561	0.00000000
Au	0.00000000	3.32554439	0.00000000

Total energy BP86/LANL2DZ: -2726.07140169

3 Molecular orbitals

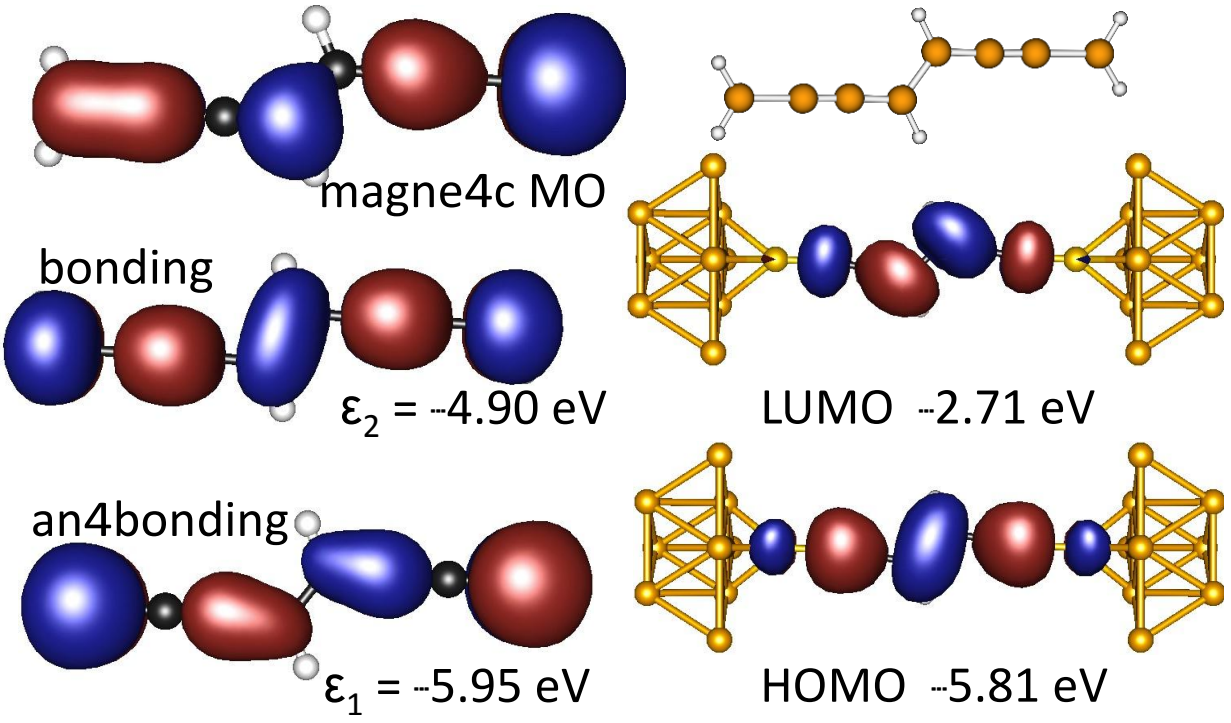


Figure 4: MO isosurface plots and energies calculated for the conjugated bridge with the "middle" C—C distance (carbon atoms 4 and 5) at the triplet optimized value. KS-DFT(BP86).

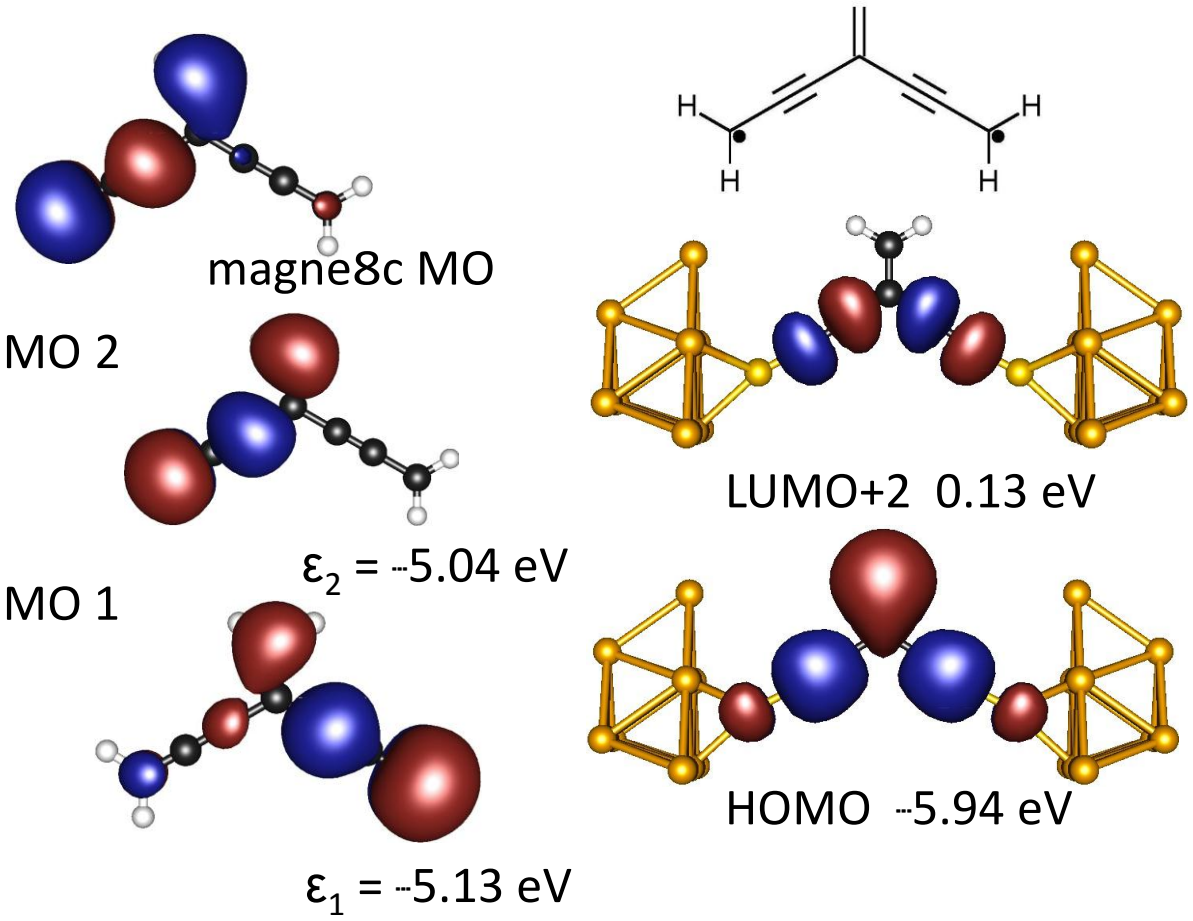


Figure 5: MO isosurface plots and energies calculated for the cross-conjugated bridge with a methylene side group. KS-DFT(BP86).

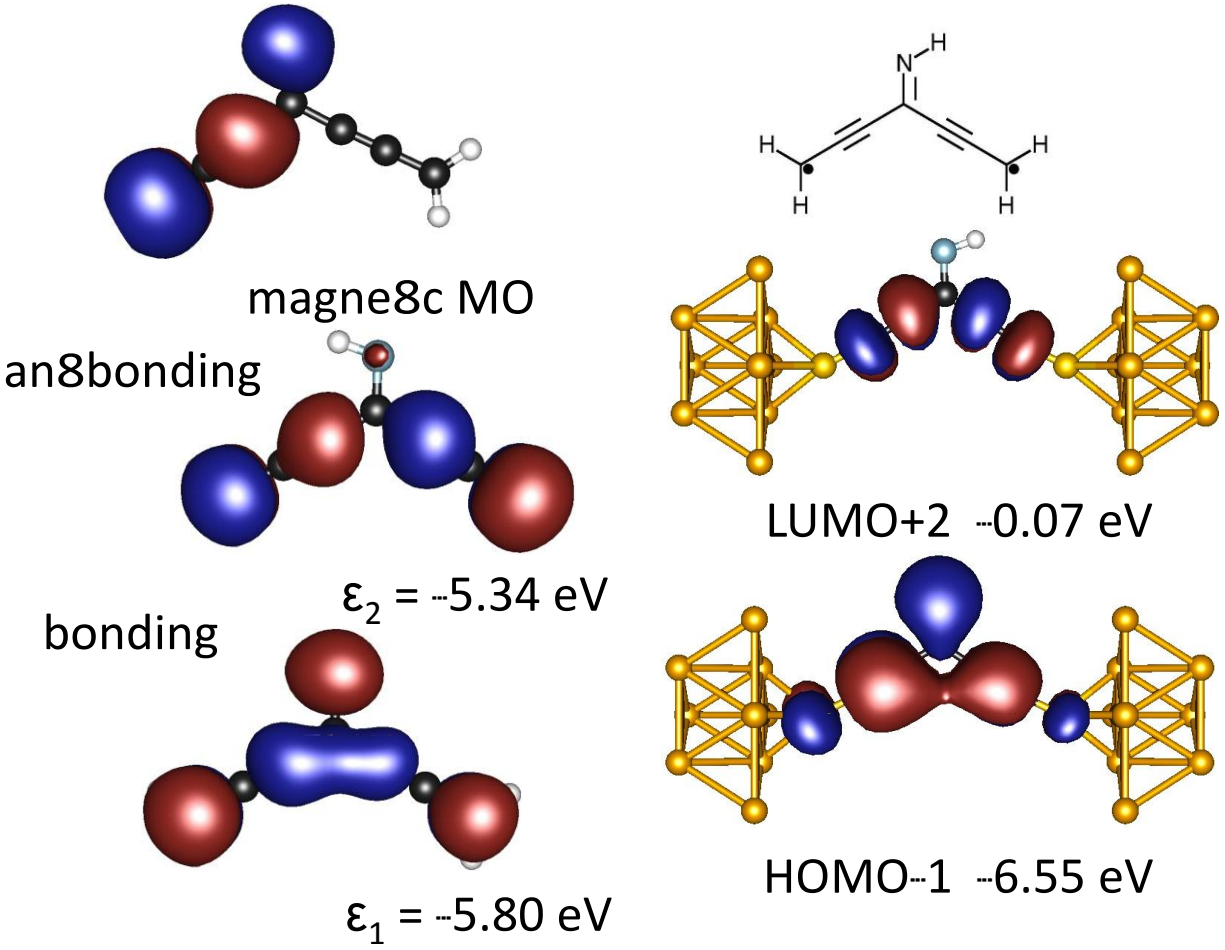


Figure 6: MO isosurface plots and energies calculated for the cross-conjugated bridge with a NH side group. KS-DFT(BP86).

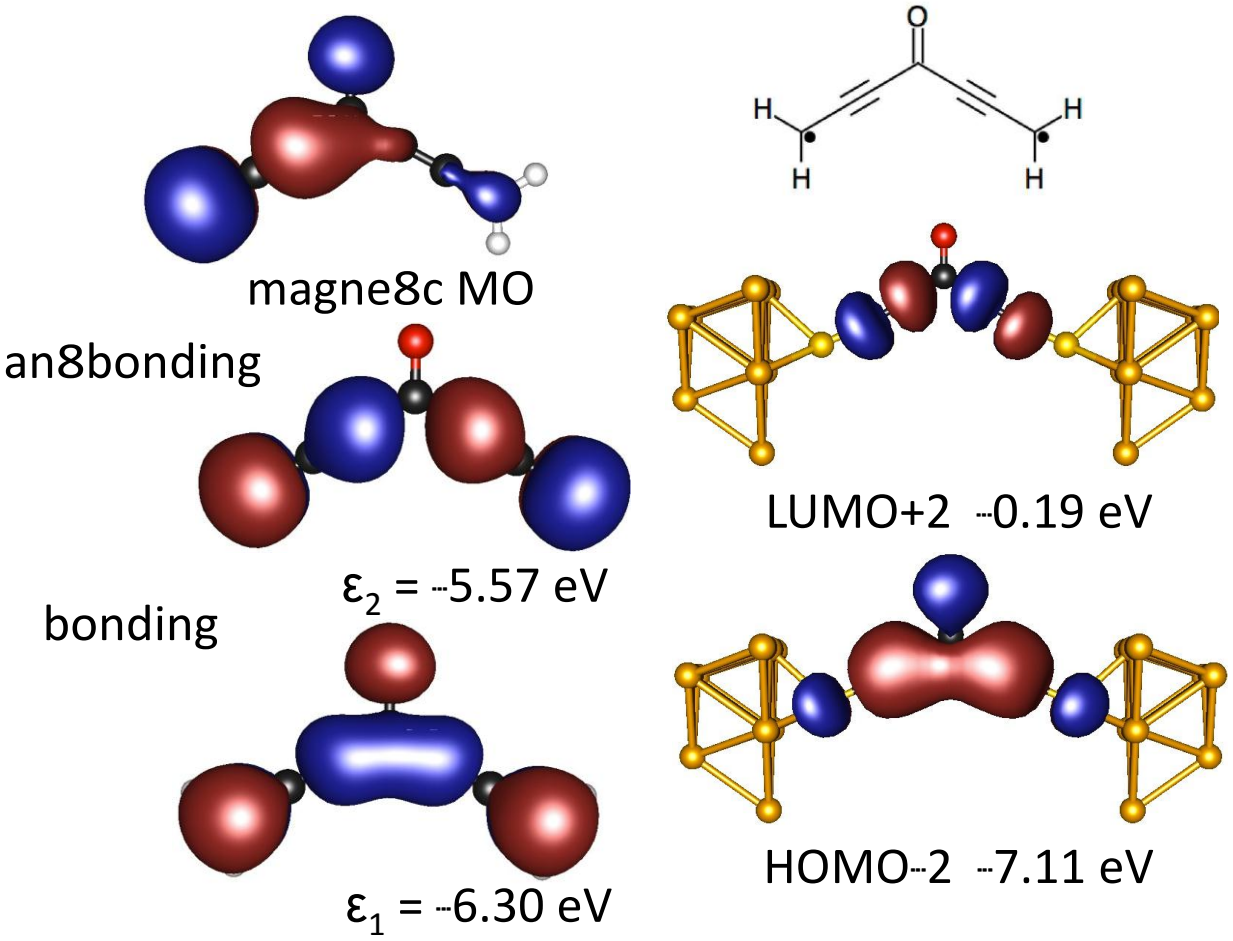


Figure 7: MO isosurface plots and energies calculated for the cross-conjugated bridge with an O side group. KS-DFT(BP86).

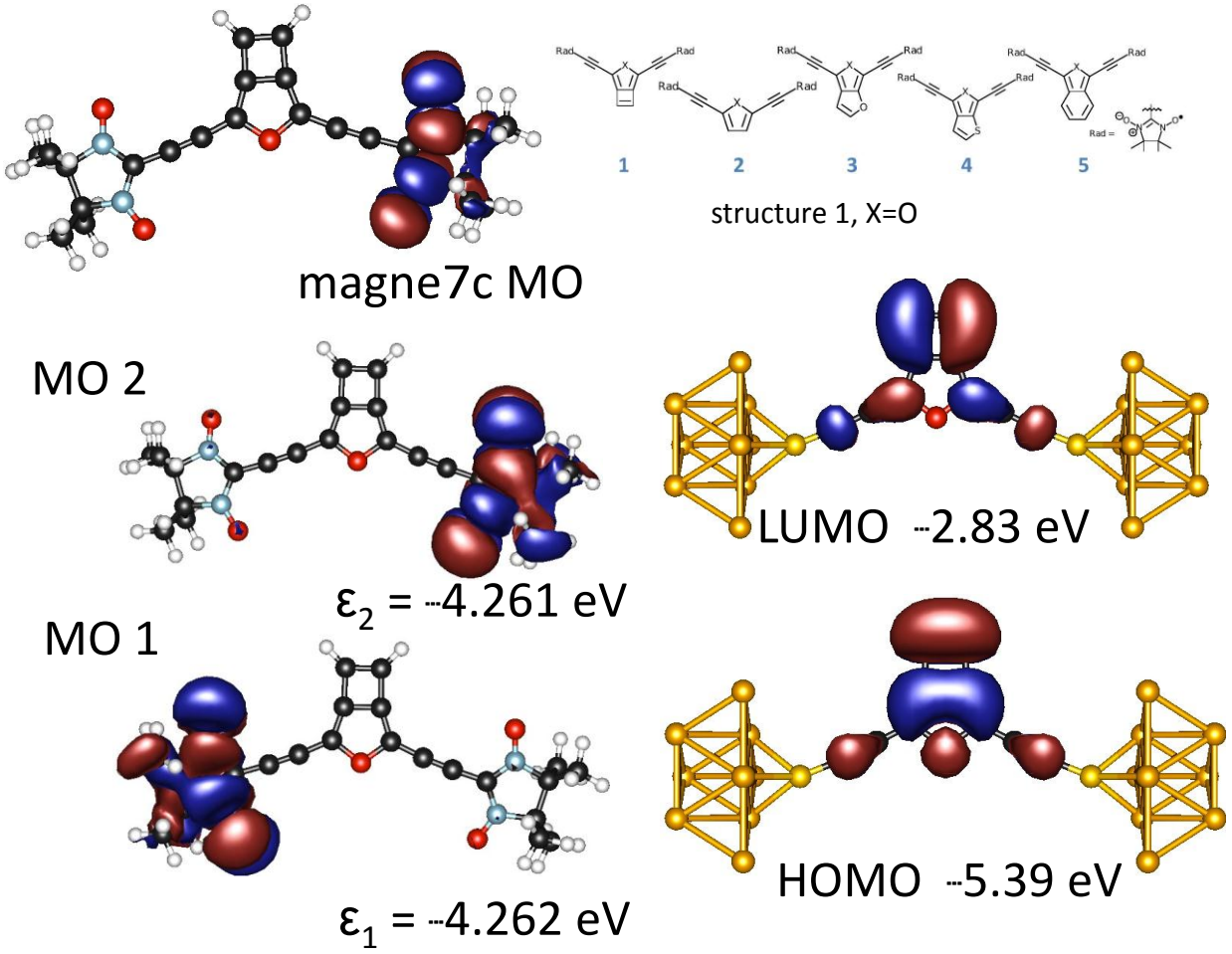


Figure 8: MO isosurface plots and energies calculated for a furane-bridge with annelated ring 1. KS-DFT(BP86).

4 Dihedral angles furane- and thiophene-bridged diradicals

Table 1: C–C^a–C^a–N dihedral angles for the furane- and thiophene-bridged diradicals, where the first two Cs are adjacent atoms of the bridging furane / thiophene ring, and the last two atoms adjacent atoms of the NNO radical group, and superscript *a* indicates that the –C≡C– spacer is attached to the marked atom. The structures are not entirely symmetric, therefore two slightly different values are obtained. The dihedral angles measure the twist between the radical plane and the bridge plane, with 0° corresponding to no twist and 90° corresponding to maximum twist.

diradical	dihedral 1	dihedral 2
X=O **1** singlet	−13.4	−14.9
X=O **1** triplet	−13.4	−14.9
X=O **2** singlet	−13.8	−16.0
X=O **2** triplet	−13.8	−16.0
X=O **4** singlet	−10.8	−14.3
X=O **4** triplet	−8.7	−14.5
X=O **5** singlet	−11.4	−14.0
X=O **5** triplet	−11.9	−15.9
X=S **1** singlet	−13.0	−14.1
X=S **1** triplet	−13.0	−14.2
X=S **2** singlet	−12.2	−14.4
X=S **2** triplet	−12.2	−14.6
X=S **4** singlet	−9.8	−14.2
X=S **4** triplet	−8.0	−13.2
X=S **5** singlet	−12.6	−13.2
X=S **5** triplet	−12.3	−12.6

5 B3LYP results for selected structures

Table 2: Different communication measures for the conjugated system shown in Figure 1 in the main manuscript. Energies in kJ/mol. KS-DFT (B3LYP). Diradical energies were obtained as single-point calculations on top of a BP86/def2-TZVP optimization of the triplet state, for which the outermost C–C bonds were elongated to 1.7 Å after optimization ("opt." in the table); for the "opt. + 0.2 Å" calculations additionally the middle C–C bond was elongated by 0.2 Å. Transport calculations were carried out on top of the BP86-optimized structures as described in the methodology section.

d(C–C)	$E_T - E_{BS}$	$T(E_F)$	$E_1 - E_2$	$E_L - E_H$
opt.	16.4	0.28	124.9	416.1
opt. + 0.2 Å	33.2	0.48	151.8	328.3

Table 3: Different communication measures for the cross-conjugated systems shown in Figure 3 in the main manuscript. Energies in kJ/mol. KS-DFT (B3LYP). Diradicals were optimized with B3LYP in their respective spin states; transport calculations were carried out on top of the BP86-optimized structures as described in the methodology section.

side group	$E_T - E_{BS}$	$T(E_F)$
$=CH_2$	−20.4	0.07
=NH	−12.6	0.08
=O	3.8	0.14

B3LYP is a hybrid functional with 20 % exact exchange admixture, while BP86 is a pure functional with no exact exchange. The B3LYP results show the same common trends for exchange spin coupling and conductance as the BP86 results.

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