

# Synthesis and properties of AABAAB-type macroheterocyclic compounds with fragments of 1,2,4- and 1,3,4-thiadiazole

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Cartesian coordinates of the optimized structure of compound **9a** yielded by B3LYP/6-31G (d, p) computations

SULFUR	16.0	-0.954101848	-5.587556784	0.477506510
NITROGEN	7.0	-0.267272516	-1.016256784	0.476071711
NITROGEN	7.0	0.097729838	1.330285968	0.963306752
NITROGEN	7.0	0.068823627	-3.241868911	-0.423979504
CARBON	6.0	-2.248183330	-5.353403967	1.641134278
CARBON	6.0	0.307359199	-1.969542939	-0.350553235
CARBON	6.0	-0.864893671	-3.825136372	0.387515207
CARBON	6.0	0.322203892	0.230363558	0.316634610
NITROGEN	7.0	-2.524585164	-4.098952311	1.864157257
CARBON	6.0	1.326853742	-1.266356342	-1.147536831
NITROGEN	7.0	-1.747325250	-3.232237929	1.163237717
CARBON	6.0	1.336143008	0.075910303	-0.739784590
CARBON	6.0	2.198470239	-1.730488635	-2.126527794
CARBON	6.0	2.216693319	0.995070814	-1.299135809
CARBON	6.0	3.081104647	-0.808236567	-2.696775908
CARBON	6.0	3.090142005	0.534427797	-2.289079139
CARBON	6.0	-2.976320335	-6.487308817	2.311841781
CARBON	6.0	-3.660992398	-6.072997414	3.633124471
SULFUR	16.0	-1.411321415	-6.643665655	5.337251128
NITROGEN	7.0	0.106313631	-3.009202662	7.744344119
NITROGEN	7.0	0.886404585	-0.862615559	8.556324774
NITROGEN	7.0	0.061972310	-5.377623667	7.230237182
CARBON	6.0	-2.717445486	-5.641285170	4.717699725
CARBON	6.0	0.532690335	-4.327767161	7.825244263
CARBON	6.0	-1.010529512	-5.280896056	6.385582011
CARBON	6.0	0.929421277	-2.154954175	8.462152798
NITROGEN	7.0	-2.787532506	-4.470413638	5.290182956
CARBON	6.0	1.707923244	-4.328555187	8.712021522
NITROGEN	7.0	-1.826686998	-4.261486937	6.227716508
CARBON	6.0	1.950309655	-3.002709070	9.101048924
CARBON	6.0	2.526205379	-5.368418284	9.138983567
CARBON	6.0	3.019003153	-2.676597025	9.928813218
CARBON	6.0	3.597058026	-5.046261600	9.978267673
CARBON	6.0	3.839658225	-3.720043300	10.367433930
SULFUR	16.0	-0.901352705	2.780604269	3.028217985
CARBON	6.0	-2.225616365	1.961666458	3.847343177
CARBON	6.0	-0.840808980	1.377066805	1.958338394
NITROGEN	7.0	-2.531536486	0.810718635	3.313251860
NITROGEN	7.0	-1.753039001	0.475823673	2.251794828
CARBON	6.0	-2.940228279	2.513845057	5.046383007
CARBON	6.0	-2.030189031	2.810726597	6.258654784
SULFUR	16.0	0.087514109	1.612525664	7.786834602
CARBON	6.0	-1.384846041	1.577165680	6.831123373
CARBON	6.0	-0.066195687	-0.144635368	7.887237499
NITROGEN	7.0	-1.870637324	0.377939822	6.670284196
NITROGEN	7.0	-1.130954713	-0.597650708	7.260222591
HYDROGEN	1.0	-1.047843656	-1.202438932	1.110355720
HYDROGEN	1.0	2.186137636	-2.772374732	-2.428844832
HYDROGEN	1.0	2.218129843	2.029471343	-0.971766511
HYDROGEN	1.0	3.773693737	-1.135313668	-3.466696816

HYDROGEN	1.0	-2.280341005	-7.316069045	2.486283703
HYDROGEN	1.0	-3.744366718	-6.874610146	1.629377493
HYDROGEN	1.0	-4.264722752	-6.920151022	3.981267457
HYDROGEN	1.0	-4.330728364	-5.228211234	3.457811146
HYDROGEN	1.0	-0.728253312	-2.708250336	7.235379671
HYDROGEN	1.0	2.331848767	-6.388947361	8.826194869
HYDROGEN	1.0	3.200996390	-1.646599750	10.217201617
HYDROGEN	1.0	4.254067769	-5.834119145	10.334598236
HYDROGEN	1.0	-3.694260755	1.772454046	5.319575152
HYDROGEN	1.0	-3.457394770	3.442436284	4.775421374
HYDROGEN	1.0	-2.635735747	3.293548868	7.037134190
HYDROGEN	1.0	-1.254333139	3.535181524	5.985193111
HYDROGEN	1.0	3.790022257	1.225419955	-2.749565259
HYDROGEN	1.0	4.681190033	-3.502026817	11.018529043

Cartesian coordinates of the optimized structure of compound **9b** yielded by B3LYP/6-31G (d, p) computations

SULFUR	16.0	-1.126765267	-5.347447826	0.665841781
NITROGEN	7.0	-0.125512705	-0.843479485	0.584501129
NITROGEN	7.0	0.104394700	1.585069026	0.699190217
NITROGEN	7.0	0.193053028	-3.126046696	-0.143911108
CARBON	6.0	-2.328749505	-5.012641396	1.896325543
CARBON	6.0	0.458354528	-1.855479198	-0.162148831
CARBON	6.0	-0.772406907	-3.620144281	0.686195664
CARBON	6.0	0.395325865	0.414103761	0.256697176
NITROGEN	7.0	-2.394402889	-3.752340553	2.229992015
CARBON	6.0	1.460727255	-1.216262020	-1.024500677
NITROGEN	7.0	-1.519393750	-2.960534255	1.550937942
CARBON	6.0	1.416331836	0.162829707	-0.776506271
CARBON	6.0	2.342172483	-1.756951025	-1.955480150
CARBON	6.0	2.252620070	1.045997092	-1.450577205
CARBON	6.0	3.185293525	-0.873350444	-2.634796237
CARBON	6.0	3.140391878	0.507383898	-2.386478049
CARBON	6.0	-3.231235853	-6.067073367	2.475174201
CARBON	6.0	-3.774234146	-5.713911115	3.878867153
SULFUR	16.0	-1.594643304	-4.631625930	5.422667015
NITROGEN	7.0	0.213997505	-3.206906863	7.601795758
NITROGEN	7.0	0.973269114	-1.004821924	8.248133314
NITROGEN	7.0	0.060046012	-5.642008763	7.485397841
CARBON	6.0	-2.758737139	-5.861160075	4.974713788
CARBON	6.0	0.581848412	-4.531532305	7.867860178
CARBON	6.0	-0.994365602	-5.802211340	6.632053171
CARBON	6.0	1.044672789	-2.300935506	8.243835374
NITROGEN	7.0	-2.646098545	-6.960978326	5.673215415
CARBON	6.0	1.765748039	-4.445914564	8.741791324
NITROGEN	7.0	-1.649884577	-6.942441705	6.592551468
CARBON	6.0	2.052889402	-3.091541252	8.961927097
CARBON	6.0	2.546105610	-5.450940639	9.302789339
CARBON	6.0	3.129545333	-2.698010963	9.750520072
CARBON	6.0	3.628916523	-5.060595428	10.096045598
CARBON	6.0	3.917197632	-3.704566322	10.315703966
SULFUR	16.0	-1.364713169	0.811462539	2.993249441
CARBON	6.0	-2.261246523	2.194442123	3.586086208
CARBON	6.0	-0.783298166	1.889898649	1.691907511
NITROGEN	7.0	-2.094823886	3.269850267	2.860865160
NITROGEN	7.0	-1.255753799	3.112449571	1.807717133
CARBON	6.0	-3.111354648	2.192476189	4.823630124
CARBON	6.0	-2.315640388	2.446862915	6.124388163
SULFUR	16.0	-0.101578169	1.398476867	7.614329341
CARBON	6.0	-1.507651743	1.261824869	6.577374287
CARBON	6.0	-0.017421815	-0.362297308	7.561768665
NITROGEN	7.0	-1.809980022	0.029482894	6.271162962
NITROGEN	7.0	-0.973639717	-0.892505111	6.823186318
HYDROGEN	1.0	-0.886543152	-1.072908134	1.224274843

HYDROGEN	1.0	2.367093313	-2.825869322	-2.138919563
HYDROGEN	1.0	2.206919898	2.111117512	-1.249777458
HYDROGEN	1.0	3.887508104	-1.259375521	-3.367694805
HYDROGEN	1.0	-2.710032985	-7.029152835	2.512956574
HYDROGEN	1.0	-4.083928593	-6.200924959	1.796020728
HYDROGEN	1.0	-4.582338755	-6.411254709	4.117278359
HYDROGEN	1.0	-4.183388448	-4.700860108	3.865515536
HYDROGEN	1.0	-0.588709579	-2.859749512	7.076245352
HYDROGEN	1.0	2.311651368	-6.495148163	9.125267267
HYDROGEN	1.0	3.341740241	-1.646726741	9.913968097
HYDROGEN	1.0	4.259460095	-5.818422504	10.551430712
HYDROGEN	1.0	-3.663320039	1.253821777	4.913544948
HYDROGEN	1.0	-3.831114488	3.006362138	4.698944945
HYDROGEN	1.0	-3.025392771	2.704985229	6.921761626
HYDROGEN	1.0	-1.665384619	3.318029034	5.994067483
HYDROGEN	1.0	3.808009063	1.167509769	-2.932216207
HYDROGEN	1.0	4.766802700	-3.435070014	10.936006993

Energies of the optimized structures of **9a** and **9b** yielded by B3LYP/6-31G (d, p) computations:

TOTAL ENERGY = -3435.7844264500 a.u.

TOTAL ENERGY = -3435.7746562082 a.u.