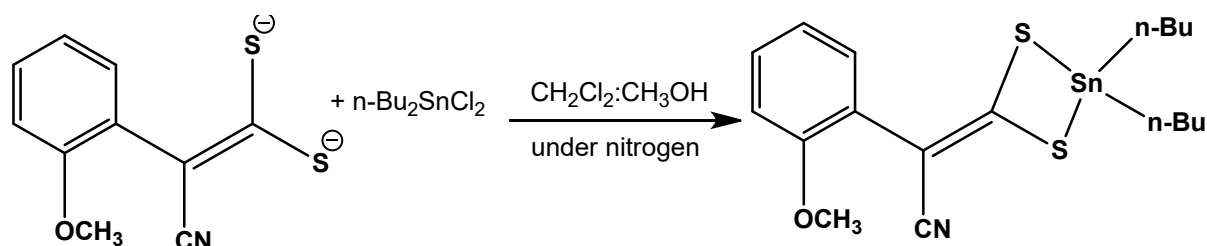


ELECTRONIC SUPPORTING INFORMATION

Unprecedented cyclization of 2-cyanobenzyl-nitrile-dithiolate to di-*n*-butyltin(IV)-bis-(1-alkoxy-isoquinoline-4-nitrile thiolate): Crystallographic and Computational Studies

Amita Singh,^{a,b} Ayushi Singh,^b Gabriele Kociok-Köhn,^c Randolph D. Köhn,^{*d} Abhinav Kumar^{*b} and Mohd. Muddassir^e



Scheme S1 Synthetic route for the preparation of methoxy-analogue.

Optimized Coordinates for Monomer of Sn-Me

Sn	4.92596719	11.28873683	-3.67505150
S	6.64317563	11.99851746	-5.15798752
S	3.04638393	12.72694711	-3.83577365
O	8.38626239	8.32485996	-2.35962477
O	1.93175384	9.13531619	-0.62834435
N	9.70480738	13.29663582	-6.49374174
N	7.68970854	9.98985400	-3.73463305
N	-0.16035872	14.18488223	-4.29585847
N	2.34661983	10.87810071	-2.02598267
C	5.61543360	11.35877027	-1.60502376
H	6.18804720	10.48699521	-1.39046935
H	4.75510140	11.39358880	-0.95185536
C	6.57771600	12.54056946	-1.37796558
H	6.88821188	12.52057620	-0.35647838
H	7.40219662	12.37092273	-2.02579572
C	6.06364017	13.95301655	-1.66980638
H	5.31263028	14.24829199	-0.96542724
H	5.65121330	14.02950829	-2.65171378
C	7.33303906	14.82151065	-1.55806136
H	7.75829315	14.70424580	-0.58132548
H	8.04116009	14.48481096	-2.29523467
H	7.10331104	15.84978267	-1.72725250
C	4.40972937	9.22022566	-4.17083319
H	3.95061545	8.76974029	-3.32312075
H	5.31855801	8.68727899	-4.41555628
C	3.34865047	9.13240031	-5.30786605
H	3.12445533	8.09754621	-5.46423147
H	2.49819193	9.65068723	-4.93837997
C	3.69204911	9.74485542	-6.69190012
H	2.79738173	9.73695939	-7.27272147
H	4.03670016	10.74933585	-6.56995734
C	4.73854112	8.91713128	-7.45391861

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H	5.66730270	8.92646289	-6.93451479
H	4.38678960	7.90573319	-7.54795129
H	4.86672695	9.34093057	-8.43384400
C	8.00523515	10.99780976	-4.60491089
C	9.26818812	11.25718065	-5.03337359
C	9.48023321	12.38343758	-5.83414758
C	10.30600776	10.39879321	-4.66882921
C	11.58388434	10.55378605	-5.15923721
H	11.80539876	11.37211386	-5.82734913
C	12.53741118	9.66925227	-4.79798727
H	13.52488642	9.77524692	-5.19712750
C	12.26100320	8.64867098	-3.94309478
H	13.04011308	7.95248309	-3.67226748
C	11.01970573	8.49543188	-3.43200309
H	10.81491789	7.69639221	-2.75479367
C	10.02078172	9.37254558	-3.79843350
C	8.61027668	9.21803666	-3.26365277
C	7.04363103	8.05356735	-1.93738372
H	7.00401898	7.07929613	-1.50045711
H	6.73537156	8.78424110	-1.21373282
H	6.38162081	8.09495265	-2.78144291
C	1.88786640	11.90841721	-2.78842503
C	0.60003976	12.30094938	-2.76925135
C	0.18523632	13.33641513	-3.60930504
C	-0.27403044	11.66044835	-1.90113270
C	-1.59628464	12.05190982	-1.79878884
H	-1.95701912	12.87215680	-2.39213911
C	-2.41400655	11.41063059	-0.93640092
H	-3.43730620	11.71145516	-0.85915925
C	-1.93467897	10.34847513	-0.15761896
H	-2.58849481	9.85225532	0.52902048
C	-0.64461102	9.95994969	-0.25222516
H	-0.27563795	9.15704990	0.35086237
C	0.20294535	10.59938622	-1.14430663
C	1.53837856	10.19706283	-1.26663312
C	3.30671435	8.72794456	-0.65217754
H	3.49751596	8.08935032	0.18430843
H	3.51054403	8.19564991	-1.56329745
H	3.94304165	9.58982658	-0.59767633

Optimized Coordinates for Dimer of Sn-Me held by C···H interactions

Sn	4.93103598	11.29149015	-3.66504326
S	6.67592396	12.03236631	-5.12419812
S	3.01557177	12.70102986	-3.86961836
O	8.38085264	8.32395412	-2.35495817
O	1.93929380	9.13349821	-0.62492782
N	9.69487285	13.28890238	-6.48241614
N	7.70355381	10.01118177	-3.71885893
N	-0.13570064	14.18044140	-4.28953163
N	2.32781279	10.86894604	-2.03844093
C	5.55772520	11.38736726	-1.56768801
H	6.11685991	10.52259017	-1.33114851
H	4.68195118	11.42842389	-0.91769750
C	6.52928086	12.57569872	-1.37013585
H	6.86229153	12.59011461	-0.35577642
H	7.33216160	12.38383952	-2.03122720

ELECTRONIC SUPPORTING INFORMATION

C	6.05071200	13.96989921	-1.66491354
H	5.31512638	14.28382925	-0.95519170
H	5.62433075	14.05449162	-2.64121226
C	7.37053478	14.78651998	-1.56276737
H	7.81115495	14.62779890	-0.59737766
H	8.05313144	14.43385380	-2.31786190
H	7.18986814	15.82156953	-1.70567369
C	4.48308834	9.19572140	-4.17211501
H	4.05242973	8.72453736	-3.32089457
H	5.41061455	8.67373799	-4.42317237
C	3.38362101	9.11987727	-5.31293129
H	3.15383710	8.08915470	-5.50495072
H	2.54456552	9.62173116	-4.90080208
C	3.67331349	9.75875431	-6.70427264
H	2.75439705	9.75483131	-7.26000684
H	4.00721473	10.77333614	-6.59352413
C	4.71023239	8.90787046	-7.48810303
H	5.66120898	8.93168373	-7.00570308
H	4.35894240	7.89506538	-7.53397504
H	4.80827744	9.29430652	-8.48359162
C	8.00818836	11.01760429	-4.57649662
C	9.26105100	11.26638383	-5.01155694
C	9.48514543	12.38242755	-5.82006261
C	10.29631284	10.40643921	-4.66105200
C	11.56689354	10.56910517	-5.16726159
H	11.77011938	11.39600850	-5.83559491
C	12.52197032	9.67241903	-4.80703734
H	13.50536915	9.76976477	-5.20720623
C	12.23467617	8.64278135	-3.93956959
H	13.00163954	7.94762972	-3.66285414
C	10.99258254	8.48990768	-3.42698685
H	10.75928125	7.69231311	-2.74617085
C	10.01874338	9.37421267	-3.79597036
C	8.61758259	9.22689609	-3.26009540
C	7.05762948	8.05246048	-1.93851155
H	7.02414357	7.09418035	-1.47131101
H	6.74819486	8.80121723	-1.24516628
H	6.40796448	8.05911268	-2.78598903
C	1.87700900	11.88729905	-2.80402483
C	0.60444304	12.28632677	-2.77722007
C	0.19731884	13.32831659	-3.60918641
C	-0.27047743	11.66149773	-1.90659826
C	-1.58630076	12.07162057	-1.81333048
H	-1.93409587	12.90641845	-2.41133848
C	-2.40269414	11.41889670	-0.94880371
H	-3.42392755	11.71312403	-0.87587623
C	-1.91265045	10.34451340	-0.15662869
H	-2.56582394	9.84092421	0.52767141
C	-0.61687745	9.95668204	-0.24432883
H	-0.22512329	9.15586458	0.36319042
C	0.20618624	10.60010691	-1.14174352
C	1.53168386	10.19811276	-1.26877659

ELECTRONIC SUPPORTING INFORMATION

C	3.30629535	8.72097466	-0.64895792
H	3.48663528	8.05109295	0.16282384
H	3.50833822	8.22455001	-1.57400210
H	3.94538879	9.57269845	-0.55604184
Sn	19.86070012	11.94498509	-11.13229663
S	21.60478771	11.20334958	-12.59184247
S	17.94536832	10.53547623	-11.33688385
O	23.31071538	14.91255272	-9.82224007
O	16.86912762	14.10300188	-8.09221786
N	24.61683148	9.94571516	-13.94931986
N	22.63267409	13.22474530	-11.18629715
N	14.79402244	9.05606782	-11.75677868
N	17.25764834	12.36755262	-9.50573244
C	20.48755606	11.84913845	-9.03497834
H	21.04670140	12.71390784	-8.79844543
H	19.61179033	11.80808165	-8.38498097
C	21.45911486	10.66080174	-8.83742766
H	21.79212581	10.64638556	-7.82306679
H	22.26199535	10.85265989	-9.49851790
C	20.98054577	9.26660077	-9.13220353
H	20.24496038	8.95267080	-8.42248165
H	20.55416471	9.18200829	-10.10850223
C	22.30036876	8.44998001	-9.03005733
H	22.74098896	8.60870111	-8.06466766
H	22.98296543	8.80264620	-9.78515190
H	22.11970214	7.41493047	-9.17296368
C	19.41291563	14.04078373	-11.63939433
H	18.98227184	14.51197158	-10.78818288
H	20.34045141	14.56275516	-11.89046517
C	18.31345414	14.11662498	-12.78021927
H	18.08367138	15.14734544	-12.97224147
H	17.47439915	13.61476954	-12.36809199
C	18.60314751	13.47774541	-14.17156240
H	17.68423103	13.48166856	-14.72729702
H	18.93704866	12.46316374	-14.06081423
C	19.64006639	14.32862939	-14.95539320
H	20.59104295	14.30481628	-14.47299325
H	19.28877627	15.34143445	-15.00126534
H	19.73811149	13.94219331	-15.95088179
C	22.93824925	12.21803810	-12.04458679
C	24.19562174	11.97126161	-12.47914452
C	24.42244887	10.85598325	-13.28753377
C	25.22593170	12.83092860	-12.12776120
C	26.49603931	12.66757736	-12.63410035
H	26.69964637	11.84049544	-13.30286220
C	27.45150427	13.56414657	-12.27436489
H	28.43514121	13.46665632	-12.67448903
C	27.16450986	14.59362641	-11.40682552
H	27.93147834	15.28886456	-11.13015892
C	25.92224041	14.74664149	-10.89437365
H	25.68919413	15.54416057	-10.21345323
C	24.94782627	13.86235668	-11.26289957

ELECTRONIC SUPPORTING INFORMATION

C	23.54713030	14.00960233	-10.72739216
C	21.98746881	15.18404169	-9.40580172
H	21.95397642	16.14231807	-8.93860108
H	21.67802825	14.43528058	-8.71245798
H	21.33779965	15.17738526	-10.25328041
C	16.80684164	11.34919645	-10.27131606
C	15.53413849	10.95018332	-10.24445476
C	15.12738018	9.90816641	-11.07656501
C	14.65936263	11.57500545	-9.37388749
C	13.34353582	11.16487974	-9.28061982
H	12.99573908	10.33008198	-9.87862922
C	12.52714060	11.81760433	-8.41609498
H	11.50590678	11.52337564	-8.34316629
C	13.01718384	12.89198575	-7.62391811
H	12.36401000	13.39557599	-6.93961891
C	14.31295682	13.27981906	-7.71162028
H	14.70471053	14.08063530	-7.10409949
C	15.13602243	12.63639330	-8.60903283
C	16.46151890	13.03838770	-8.73606744
C	18.23612937	14.51552537	-8.11624813
H	18.41646934	15.18540720	-7.30446651
H	18.43817226	15.01194983	-9.04129239
H	18.87522287	13.66380158	-8.02333188

Optimized coordinates for the Dimer of Sn-Me held by N $\cdots$ H and C $\cdots$ H interactions

Sn	7.79713340	4.20618138	3.65900399
S	6.05556365	3.45807842	5.11485899
S	9.71178984	2.79822732	3.87481386
O	4.34890551	7.16774538	2.36020286
O	10.78829090	6.35201172	0.62179900
N	3.03532086	2.20003858	6.48593709
N	5.02551754	5.47928880	3.71556803
N	12.86655779	1.30556909	4.29132919
N	10.40004240	4.62622082	2.04118152
C	7.16749129	4.09537128	1.56154833
H	6.61221245	4.96008352	1.31546686
H	8.04408411	4.03751249	0.91799610
C	6.19726891	2.91414759	1.36917373
H	5.86312051	2.90045712	0.35400750
H	5.39209366	3.10593089	2.03426401
C	6.67759270	1.52104831	1.66460857
H	7.41351309	1.20177133	0.95380114
H	7.10500468	1.43300691	2.64258227
C	5.36287399	0.71181457	1.56296393
H	4.92493195	0.87605000	0.59659540
H	4.68441415	1.06486405	2.32061142
H	5.54054053	-0.32512133	1.70171343
C	8.24895189	6.29737384	4.17982505
H	8.67771356	6.77621743	3.33296543
H	7.32320636	6.80833852	4.44473617
C	9.34427817	6.37296987	5.31242244

ELECTRONIC SUPPORTING INFORMATION

H	9.57210966	7.40365985	5.50360887
H	10.18582233	5.86683027	4.90407635
C	9.05210362	5.73656662	6.70108358
H	9.97163428	5.73914002	7.25712442
H	8.71265185	4.72448869	6.58827011
C	8.02248417	6.58257959	7.48697465
H	7.06972378	6.55260722	7.00862082
H	8.36922350	7.59778703	7.52855203
H	7.93273854	6.19739231	8.48378404
C	4.73077248	4.47047965	4.56919717
C	3.47682809	4.22100371	5.00927681
C	3.24005187	3.10743872	5.82157173
C	2.44493364	5.08003652	4.66023058
C	1.16806310	4.92242633	5.16603117
H	0.95387209	4.10413626	5.82990523
C	0.20926480	5.82009070	4.80684720
H	-0.77332414	5.72415710	5.20492240
C	0.49304507	6.84884570	3.93873355
H	-0.27085909	7.54067258	3.66337196
C	1.73450333	7.00149988	3.42819409
H	1.96552869	7.79784446	2.74748844
C	2.71524372	6.11388535	3.79783965
C	4.10906333	6.26398671	3.26253076
C	5.67075861	7.43776009	1.94024667
H	5.70301000	8.39638800	1.46840982
H	5.97716092	6.68608784	1.24842930
H	6.32115229	7.43497658	2.78759825
C	10.84524726	3.60918797	2.80926742
C	12.11958655	3.20585691	2.77998729
C	12.53068839	2.16021470	3.61158529
C	12.99132068	3.83114901	1.91214775
C	14.31152625	3.41910909	1.80933013
H	14.66599368	2.59196044	2.40218140
C	15.13222777	4.07519302	0.94996534
H	16.15392977	3.78272841	0.87455038
C	14.64247927	5.14421905	0.15466262
H	15.29551155	5.64778384	-0.52548734
C	13.34868572	5.53315008	0.24630568
H	12.96242063	6.33223573	-0.36102933
C	12.51559227	4.88591779	1.14190814
C	11.19828332	5.29213092	1.26967372
C	9.42322620	6.76877803	0.64873118
H	9.24336151	7.44420015	-0.16175976
H	9.22622109	7.26213044	1.57593375
H	8.78221963	5.91878881	0.55192342
Sn	5.59689368	3.53936980	11.12626994
S	3.85574364	4.28823677	12.58257509
S	7.51146344	4.94726309	11.34205304
O	2.14847233	0.57773615	9.82750292
O	8.58785714	1.39348811	8.08908914
N	0.83874490	5.54633436	13.95304942
N	2.82568869	2.26683091	11.18308451

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N	10.66795572	6.43977588	11.75790881
N	8.19960913	3.11927715	9.50846950
C	4.96706612	3.65012257	9.02883890
H	4.41176646	2.78541890	8.78276911
H	5.84364169	3.70797743	8.38527440
C	3.99683520	4.83135136	8.83646623
H	3.66268587	4.84504247	7.82129825
H	3.19166019	4.63957002	9.50155540
C	4.47715904	6.22445164	9.13189862
H	5.21307911	6.54372856	8.42109106
H	4.90457078	6.31249325	10.10987223
C	3.16244004	7.03368544	9.03025387
H	2.72449794	6.86944999	8.06388539
H	2.48398016	6.68063596	9.78790142
H	3.34010653	8.07062133	9.16900340
C	6.04853040	1.44812147	11.64710195
H	6.47726654	0.96926750	10.80025225
H	5.12276776	0.93717338	11.91202935
C	7.14384595	1.37252621	12.77970894
H	7.37167525	0.34183974	12.97089997
H	7.98538917	1.87866830	12.37136604
C	6.85166949	2.00893358	14.16837300
H	7.77120027	2.00636018	14.72441454
H	6.51221786	3.02101139	14.05556003
C	5.82205014	1.16292056	14.95426475
H	4.86928980	1.19289273	14.47591100
H	6.16878962	0.14771310	14.99584237
H	5.73230449	1.54810788	15.95107419
C	2.52829540	3.27502445	12.03701523
C	1.27401941	3.52389683	12.47677114
C	1.03795792	4.63766890	13.28883241
C	0.24278172	2.66463728	12.12730658
C	-1.03213972	2.82261758	12.63286917
H	-1.24609538	3.64131430	13.29710638
C	-1.99087131	1.92537749	12.27405293
H	-2.97363453	2.02143124	12.67224345
C	-1.70730499	0.89666764	11.40610904
H	-2.47131107	0.20486652	11.13065422
C	-0.46562564	0.74396547	10.89542314
H	-0.23499454	-0.05234500	10.21480124
C	0.51530352	1.63145902	11.26485870
C	1.90920633	1.48161503	10.72976572
C	3.47031276	0.30773258	9.40752914
H	3.50257740	-0.65088587	8.93569953
H	3.77672761	1.05941528	8.71572162
H	4.12071496	0.31052606	10.25489055
C	8.64509102	4.13620043	10.27636014
C	9.91956468	4.53960507	10.24712840
C	10.32734590	5.58554119	11.08000750
C	10.79121308	3.91441077	9.37938610
C	12.11112863	4.32637760	9.27659740
H	12.46555749	5.15353812	9.86947017

ELECTRONIC SUPPORTING INFORMATION

C	12.93179465	3.67030633	8.41725339
H	13.95349537	3.96277186	8.34184084
C	12.44204495	2.60128117	7.62195277
H	13.09507761	2.09771607	6.94180292
C	11.14824486	2.21234712	7.71359486
H	10.76198692	1.41326410	7.10626072
C	10.31517002	2.85958770	8.60920173
C	8.99783809	2.45337004	8.73696739
C	7.22279225	0.97672184	8.11602134
H	7.04292745	0.30129970	7.30553058
H	7.02578706	0.48336974	9.04322405
H	6.58178557	1.82671118	8.01921347

Optimized coordinates of Dimer of Sn-Me held by O $\cdots$ H interactions

Sn	7.79982234	4.19965483	3.66542641
S	6.05470806	3.45440099	5.12818868
S	9.71525778	2.78709855	3.87120273
O	4.34447583	7.16666179	2.35643066
O	10.79248811	6.35610361	0.62413119
N	3.04053190	2.19952180	6.48143617
N	5.02928908	5.48023785	3.71910050
N	12.86308253	1.31105518	4.29072669
N	10.39982279	4.62165420	2.03747639
C	7.16806575	4.10482482	1.56651844
H	6.61466756	4.96837333	1.33430034
H	8.05283285	4.06632576	0.91493147
C	6.20426132	2.91431157	1.37071700
H	5.86676008	2.89804331	0.35575266
H	5.39845496	3.10736366	2.03128185
C	6.67726899	1.52650892	1.66284381
H	7.41483104	1.20697345	0.95573494
H	7.10589536	1.43505436	2.64153803
C	5.35842039	0.70407582	1.56436862
H	4.91630933	0.86250141	0.59646497
H	4.67418722	1.05690484	2.31830489
H	5.53791836	-0.33257791	1.70563363
C	8.24645301	6.29592110	4.17071820
H	8.67512631	6.76407402	3.31940955
H	7.31316279	6.82118750	4.42002292
C	9.34476118	6.37181601	5.31013433
H	9.57749638	7.40229222	5.50823083
H	10.18471816	5.86950988	4.90010969
C	9.05439953	5.73259700	6.70358693
H	9.97756275	5.73459745	7.26080000
H	8.72565239	4.71386316	6.59550460
C	8.02004217	6.58322655	7.48921261
H	7.06634128	6.56074697	7.00574803
H	8.37122467	7.59719150	7.53409191
H	7.92016152	6.19669689	8.48484511
C	4.71352840	4.47253293	4.57638032
C	3.45972144	4.23021100	5.01572585
C	3.24069081	3.11165935	5.81885318

ELECTRONIC SUPPORTING INFORMATION

C	2.42923261	5.08263503	4.65745763
C	1.16534095	4.92153365	5.16949434
H	0.96040926	4.09228165	5.83657474
C	0.20870703	5.81839886	4.80971686
H	-0.77627212	5.72122476	5.20680420
C	0.49148616	6.84663377	3.93509182
H	-0.27076254	7.54455509	3.66392259
C	1.73777436	7.00388695	3.42848889
H	1.97181731	7.79774902	2.74603361
C	2.71483348	6.11728365	3.79445616
C	4.11365799	6.26511962	3.25633762
C	5.67236162	7.43754307	1.93805938
H	5.70507515	8.39769664	1.47118235
H	5.98192811	6.68929169	1.24467777
H	6.32220105	7.43223335	2.78674643
C	10.85631202	3.60184304	2.80211377
C	12.12735802	3.20327854	2.77452297
C	12.53316823	2.16422533	3.60646948
C	13.00387790	3.83479366	1.91366599
C	14.31305418	3.41217895	1.80919425
H	14.66353154	2.58385043	2.41475126
C	15.13298241	4.07393288	0.95334504
H	16.15240115	3.77674116	0.87509864
C	14.64310442	5.14760826	0.15449745
H	15.29386672	5.65013883	-0.52745725
C	13.34795184	5.53663245	0.24364487
H	12.95138302	6.33519556	-0.36331942
C	12.51899545	4.88755764	1.13738919
C	11.19934495	5.29844048	1.27103013
C	9.42213916	6.77001837	0.65028037
H	9.24322647	7.44028979	-0.16378568
H	9.22039043	7.26709251	1.57481341
H	8.78322325	5.91761964	0.55559001
Sn	4.92967833	11.29133038	-3.66545188
S	6.67524812	12.03615134	-5.12794205
S	3.01416286	12.70390684	-3.87121868
O	8.38490652	8.32435758	-2.35641988
O	1.93691188	9.13489639	-0.62413119
N	9.69163742	13.29118790	-6.48103451
N	7.70056089	10.01046731	-3.71895816
N	-0.13399917	14.17993353	-4.29058717
N	2.32957869	10.86934562	-2.03747727
C	5.56133564	11.38617957	-1.56651831
H	6.11472822	10.52262531	-1.33429655
H	4.67656429	11.42467720	-0.91493509
C	6.52513877	12.57668848	-1.37071597
H	6.86263975	12.59295677	-0.35575248
H	7.33094519	12.38363603	-2.03128149
C	6.05213112	13.96449105	-1.66284384
H	5.31456896	14.28402656	-0.95573498
H	5.62350466	14.05594559	-2.64153805
C	7.37097962	14.78692417	-1.56436865

ELECTRONIC SUPPORTING INFORMATION

H	7.81309066	14.62849859	-0.59646497
H	8.05521279	14.43409516	-2.31830489
H	7.19148163	15.82357790	-1.70563363
C	4.48295035	9.19508191	-4.17072379
H	4.05426917	8.72693085	-3.31941066
H	5.41623566	8.66980878	-4.42002137
C	3.38463932	9.11918519	-5.31013560
H	3.15190343	8.08870782	-5.50823055
H	2.54468202	9.62149044	-4.90010980
C	3.67500046	9.75840283	-6.70358715
H	2.75183727	9.75640252	-7.26080001
H	4.00374765	10.77713678	-6.59550459
C	4.70935783	8.90777341	-7.48921264
H	5.66305873	8.93025299	-7.00574804
H	4.35817535	7.89380847	-7.53409193
H	4.80923848	9.29430311	-8.48484511
C	8.01533337	11.01807126	-4.57610160
C	9.26672399	11.26204033	-5.01476977
C	9.48719742	12.37902822	-5.81996267
C	10.29979141	10.40860442	-4.65807106
C	11.56450066	10.56975929	-5.16955091
H	11.76915361	11.39867825	-5.83664329
C	12.52084440	9.67256544	-4.80979783
H	13.50571230	9.76974307	-5.20678902
C	12.23792376	8.64434743	-3.93506118
H	13.00015848	7.94643818	-3.66392005
C	10.99170979	8.48706919	-3.42853072
H	10.75753949	7.69324877	-2.74601938
C	10.01507569	9.37390818	-3.79445101
C	8.61589647	9.22580575	-3.25642446
C	7.05703602	8.05345675	-1.93805933
H	7.02432538	7.09330256	-1.47118241
H	6.74747236	8.80170720	-1.24467701
H	6.40719831	8.05876572	-2.78674582
C	1.87306550	11.88914803	-2.80209869
C	0.60186864	12.28771944	-2.77444283
C	0.19677608	13.32679348	-3.60671117
C	-0.27450747	11.65621016	-1.91366111
C	-1.58365513	12.07881989	-1.80919227
H	-1.93413153	12.90714953	-2.41475125
C	-2.40358243	11.41706713	-0.95334498
H	-3.42300115	11.71425883	-0.87509866
C	-1.91370442	10.34339173	-0.15449747
H	-2.56446672	9.84086117	0.52745725
C	-0.61855170	9.95436752	-0.24364484
H	-0.22198303	9.15580443	0.36331941
C	0.21040593	10.60344298	-1.13738963
C	1.53005525	10.19255956	-1.27103019
C	3.30726084	8.72098163	-0.65028037
H	3.48617353	8.05071021	0.16378568
H	3.50900956	8.22390749	-1.57481341
H	3.94617674	9.57338036	-0.55559001

ELECTRONIC SUPPORTING INFORMATION

Optimized Coordinates of the Sn-Et monomer

Sn	-6.69297995	3.83750330	12.17182434
S	-4.84227987	5.28709285	12.62953923
S	-8.49413809	4.36238510	13.65301201
O	-3.89294640	2.23580289	8.81191722
O	-10.22243739	0.90022916	10.73844533
N	-11.34358618	5.54790615	15.28803674
N	-9.52829710	2.50678741	12.11900240
N	-1.72484175	6.85823691	12.95521852
N	-4.19824338	3.60662833	10.57868095
C	-7.40134153	4.29756071	10.11170239
H	-8.05938751	3.51994402	9.72676509
H	-6.54326268	4.40044522	9.43338560
C	-8.26314626	5.60792686	10.20726790
H	-7.70653530	6.40141771	10.70172451
H	-9.15559643	5.37779307	10.79766535
C	-8.68721986	6.09838663	8.80065692
H	-7.80128594	6.40729640	8.26345411
H	-9.19122556	5.30169412	8.27309672
C	-9.67037668	7.29872486	8.91655451
H	-9.92100967	7.63550838	7.91433926
H	-10.57432445	6.97601098	9.43172033
H	-9.20477816	8.10604998	9.47138648
C	-6.04796383	1.72748135	12.50038661
H	-4.93219354	1.64703086	12.34035535
H	-6.56508105	1.09584673	11.82106259
C	-6.50237970	1.20577958	13.91229382
H	-7.58314842	1.35843750	13.97530839
H	-6.26477150	0.15484404	14.01697984
C	-5.84369939	1.92026408	15.08110724
H	-4.78419670	1.73824384	15.04915408
H	-6.04528923	2.97969695	15.03059867
C	-6.43008701	1.35311131	16.39989080
H	-5.94221266	1.83603388	17.23263318
H	-7.50040375	1.53822837	16.43111149
H	-6.24960004	0.27599976	16.43864158
C	-9.75812328	3.42037509	13.08105731
C	-10.97070841	3.65092020	13.59192111
C	-11.22475147	4.67477751	14.53218247
C	-11.97393920	2.86926935	13.15767742
C	-13.28645743	2.97959443	13.69159714
H	-13.52516187	3.71502836	14.42297608
C	-14.26838128	2.12728140	13.25604576
H	-15.25661902	2.19159160	13.65707367
C	-13.98864884	1.14629953	12.28000984
H	-14.75431514	0.46758904	11.97936328

ELECTRONIC SUPPORTING INFORMATION

C	-12.74341967	1.02825199	11.76575672
H	-12.53036669	0.27853601	11.03465476
C	-11.72131553	1.89801773	12.19016236
C	-10.45985964	1.77532229	11.65795226
C	-8.90273791	0.58624343	10.28007101
H	-8.94060288	0.30795554	9.23114015
H	-8.24306248	1.43947790	10.40075908
C	-8.39369843	-0.59592843	11.11452391
H	-7.40210185	-0.87432646	10.77415208
H	-8.35428800	-0.30233810	12.15970692
H	-9.07300781	-1.43551668	10.99407317
C	-3.74049982	4.56919991	11.43727262
C	-2.46598220	4.98661497	11.38957374
C	-2.05971225	6.01261053	12.24784166
C	-1.61073081	4.39858409	10.48686860
C	-0.25622707	4.77352116	10.40135723
H	0.13913534	5.55119684	11.01602656
C	0.56832246	4.13752727	9.51342720
H	1.60420771	4.39711579	9.45561242
C	0.06690609	3.13692894	8.65720663
H	0.72280475	2.64417989	7.97650564
C	-1.24273879	2.79933983	8.69664338
H	-1.62899407	2.06821300	8.02058443
C	-2.10056570	3.41997445	9.62541424
C	-3.42782642	3.07359302	9.67758031
C	-5.21123751	1.68883064	8.90522304
H	-5.39039102	1.30176208	9.90490294
H	-5.93361730	2.45392885	8.67410801
C	-5.33635849	0.56028978	7.86299457
H	-6.33845194	0.14264189	7.91105642
H	-5.16169278	0.98178147	6.87579229
H	-4.60690838	-0.21391643	8.06827706

Optimized Coordinates of the Dimer of Sn-Et held by Ar-H $\cdots\pi$ interactions

Sn	8.03370792	4.26633969	4.29755480
S	9.87294881	2.84505328	4.75267198
S	6.27561376	3.75123683	5.79051865
O	10.81893153	5.86218962	0.92010493
O	4.49095549	7.20934033	2.83701654
N	3.37696424	2.58118294	7.40055587
N	5.20513791	5.60527260	4.25388175
N	13.01495668	1.26145289	5.07049171
N	10.52735132	4.47913189	2.71143121
C	7.33670157	3.82325581	2.24972958
H	6.69293363	4.58736833	1.89047323
H	8.16831157	3.72643227	1.59694819
C	6.47645021	2.49645404	2.32701739
H	7.02962615	1.71986927	2.79520531
H	5.60489981	2.70923160	2.91263461

ELECTRONIC SUPPORTING INFORMATION

C	6.04094017	2.01471354	0.91638803
H	6.90796351	1.72555283	0.37030959
H	5.55055220	2.80468375	0.39770134
C	5.06177637	0.81371828	1.03364257
H	4.79889268	0.46915413	0.06031686
H	4.17869779	1.11902408	1.54512889
H	5.51983454	0.01931181	1.57198953
C	8.64767431	6.37823509	4.58338882
H	9.69930650	6.47827561	4.39237667
H	8.10710974	6.98805365	3.92471674
C	8.23565389	6.89089450	6.02985531
H	7.18108438	6.75834159	6.11040694
H	8.47542105	7.92795121	6.11227435
C	8.89549388	6.17130911	7.20089810
H	9.94284612	6.33388330	7.16880831
H	8.69832223	5.13324296	7.14641523
C	8.30543576	6.75115950	8.51499246
H	8.76471999	6.28399046	9.34904343
H	7.25288787	6.57400193	8.55023171
H	8.47821947	7.80176282	8.56086846
C	4.93200357	4.68615602	5.19805613
C	3.70514054	4.46481024	5.69928344
C	3.52461615	3.42806988	6.63563058
C	2.68232513	5.27242834	5.27454879
C	1.41848485	5.14529140	5.80211027
H	1.21739104	4.37928504	6.53775669
C	0.45653936	5.98516172	5.37777037
H	-0.52792647	5.90160399	5.77460434
C	0.74065013	6.96601629	4.40877046
H	-0.03154714	7.63165171	4.08457830
C	1.98229968	7.08694945	3.88857795
H	2.19294423	7.81843820	3.13873913
C	2.97531596	6.23711655	4.31919859
C	4.26782766	6.34594313	3.78627470
C	5.81298643	7.52077036	2.39218682
H	5.79084560	7.78877071	1.36641464
H	6.46102175	6.67947068	2.51624413
C	6.33549645	8.70627403	3.23190253
H	7.31074840	8.98141399	2.90758480
H	6.37741205	8.42886076	4.25947108
H	5.68112523	9.53534950	3.11823376
C	10.99467701	3.52944691	3.56323502
C	12.27627343	3.11555765	3.50644349
C	12.66557717	2.09431436	4.37445693
C	13.14616707	3.70689562	2.58664293
C	14.48451170	3.33904553	2.51190479
H	14.85525196	2.56193520	3.15241026
C	15.29774175	3.96847400	1.62958504
H	16.32680829	3.70375886	1.58261164
C	14.79098284	4.96798373	0.77528849
H	15.44643433	5.46244557	0.09079383
C	13.48425346	5.30631846	0.81390577

ELECTRONIC SUPPORTING INFORMATION

H	13.09259504	6.04933985	0.14825007
C	12.64571029	4.68192070	1.73335577
C	11.29157452	5.02149423	1.80010360
C	9.51208311	6.41468039	1.01507368
H	9.34173215	6.77934267	2.00456022
H	8.79069354	5.66324473	0.79875398
C	9.38498531	7.55276314	-0.01701669
H	8.40841760	7.96828907	0.02499210
H	9.55828963	7.15834748	-0.99124978
H	10.09925617	8.31177932	0.18669628
Sn	-6.69171902	3.84197271	12.17967808
S	-4.85257302	5.26308420	12.63464695
S	-8.44978738	4.35713732	13.67268361
O	-3.90644917	2.24616376	8.80223243
O	-10.23450454	0.89900971	10.71918960
N	-11.34777695	5.52736835	15.28264406
N	-9.52032337	2.50307640	12.13605561
N	-1.70367118	6.84794342	12.94813090
N	-4.19814444	3.62899186	10.59338942
C	-7.38875176	4.28509413	10.13189753
H	-8.03253477	3.52098681	9.77265876
H	-6.55715452	4.38191572	9.47911071
C	-8.24900708	5.61189809	10.20919220
H	-7.69583396	6.38848221	10.67737810
H	-9.12055902	5.39911873	10.79480910
C	-8.68451992	6.09363668	8.79856146
H	-7.81749666	6.38279716	8.25248251
H	-9.17490781	5.30366605	8.27987457
C	-9.66368377	7.29463165	8.91581555
H	-9.92656738	7.63919583	7.94248982
H	-10.54676231	6.98932592	9.42730183
H	-9.20562553	8.08903816	9.45416250
C	-6.07777928	1.73011035	12.46555796
H	-5.02615365	1.63006112	12.27454721
H	-6.61836200	1.12029951	11.80689736
C	-6.48980454	1.21745796	13.91202969
H	-7.54437561	1.35001055	13.99258052
H	-6.25004029	0.18039927	13.99444751
C	-5.82996611	1.93704123	15.08307148
H	-4.78261410	1.77446657	15.05098125
H	-6.02713786	2.97510707	15.02858842
C	-6.42002435	1.35719049	16.39716554
H	-5.96074002	1.82435950	17.23121642
H	-7.47257220	1.53434804	16.43240482
H	-6.24724060	0.30658716	16.44304146
C	-9.79341161	3.42221844	13.08023480
C	-11.01982072	3.64368556	13.58139268
C	-11.20212001	4.67992019	14.51795592
C	-12.04310059	2.83592257	13.15671424
C	-13.30697469	2.96306069	13.68428505
H	-13.50806936	3.72906501	14.41992961
C	-14.26892099	2.12318828	13.25994334

ELECTRONIC SUPPORTING INFORMATION

H	-15.25338664	2.20674592	13.65677723
C	-13.98480997	1.14233372	12.29094334
H	-14.75700719	0.47669820	11.96675129
C	-12.74316054	1.02140053	11.77075097
H	-12.53251578	0.28991183	11.02091210
C	-11.75014691	1.87123258	12.20137202
C	-10.45763274	1.76240703	11.66844809
C	-8.91247358	0.58757964	10.27435985
H	-8.93461443	0.31957930	9.24858765
H	-8.26443828	1.42887933	10.39841715
C	-8.38996355	-0.59792402	11.11407553
H	-7.41471161	-0.87306398	10.78975780
H	-8.34804795	-0.32051076	12.14164409
H	-9.04433478	-1.42699950	11.00040676
C	-3.73104278	4.57851503	11.44514504
C	-2.44761703	4.99393539	11.38641382
C	-2.06897983	6.01196750	12.26356058
C	-1.57926842	4.40163538	10.46919172
C	-0.24106032	4.76949560	10.39429782
H	0.13008860	5.54653094	11.03458493
C	0.57235172	4.13992328	9.51178325
H	1.60144204	4.40456217	9.46472102
C	0.06560476	3.14038122	8.65742832
H	0.72097206	2.64588117	7.97295082
C	-1.24104713	2.80211139	8.69610191
H	-1.63288216	2.05902151	8.03043632
C	-2.07977967	3.42655770	9.61566119
C	-3.43358019	3.08683448	9.68215621
C	-5.21337634	1.69367674	8.89725745
H	-5.38372975	1.32900788	9.88673480
H	-5.93476883	2.44510559	8.68092986
C	-5.34047620	0.55558716	7.86515881
H	-6.31704249	0.14006079	7.90716441
H	-5.16717021	0.95000279	6.89092317
H	-4.62620371	-0.20342898	8.06886911

Optimized coordinates of the Dimer of Sn-Et held by N $\cdots$ H bifurcated interactions

Sn	8.03582849	4.25509101	4.30635488
S	9.88964315	2.82162708	4.75489528
S	6.24380775	3.75268315	5.78879579
O	10.82485523	5.85926653	0.91910556
O	4.49296315	7.21019981	2.84518929
N	3.38872994	2.57765166	7.40252953
N	5.19384659	5.60746880	4.24395475
N	13.00175097	1.25918157	5.07187533
N	10.53330696	4.48689987	2.70214960
C	7.33855350	3.82367322	2.24598392
H	6.67926147	4.59744710	1.88037440
H	8.18792858	3.73094455	1.57545655
C	6.47172551	2.49458766	2.33094749
H	7.02891699	1.70428904	2.80886688
H	5.58605087	2.72060041	2.91921476

ELECTRONIC SUPPORTING INFORMATION

C	6.03956225	2.01200805	0.91758588
H	6.92384452	1.71823600	0.36512690
H	5.54130945	2.81374241	0.38709601
C	5.06007430	0.81475718	1.03093526
H	4.79847173	0.46581550	0.04337602
H	4.16129501	1.12658739	1.55402142
H	5.52439021	0.00537806	1.58586957
C	8.66156465	6.37640050	4.58514258
H	9.74935911	6.47990005	4.38947926
H	8.10447726	6.98939712	3.92307057
C	8.23393961	6.89456284	6.03691988
H	7.15794521	6.75491448	6.10286252
H	8.47406892	7.94590435	6.12835366
C	8.88968404	6.17181886	7.20264436
H	9.94989999	6.34747392	7.16820803
H	8.68924624	5.12153817	7.14731269
C	8.30404911	6.75670770	8.51192530
H	8.77459109	6.27394910	9.35651262
H	7.23179787	6.56960119	8.55092104
H	8.47772119	7.82147466	8.55890876
C	4.93128525	4.69976179	5.20190136
C	3.72198972	4.46084357	5.69892151
C	3.49378348	3.43116238	6.63535303
C	2.71424002	5.26942782	5.28659597
C	1.43166609	5.12720981	5.80260158
H	1.21094730	4.37583459	6.54854779
C	0.45832064	5.98086049	5.37663433
H	-0.53518686	5.90679961	5.77885867
C	0.74058060	6.96805384	4.40839076
H	-0.03227423	7.63873589	4.08525108
C	1.98580294	7.07839372	3.87813003
H	2.19957124	7.83037181	3.14066252
C	2.98826654	6.22288129	4.30846678
C	4.26441416	6.34336177	3.78364688
C	5.81594473	7.51768565	2.39220260
H	5.78342021	7.79212676	1.35251305
H	6.47330788	6.66600762	2.51710743
C	6.33647178	8.70662540	3.23396977
H	7.32389288	8.98502861	2.89988435
H	6.37512256	8.42172582	4.27733410
H	5.66431711	9.54729045	3.11572062
C	10.99968206	3.53089235	3.55878807
C	12.26496132	3.12095121	3.50975988
C	12.68041878	2.09693138	4.36323984
C	13.13367507	3.71096958	2.59783311
C	14.47712746	3.33383464	2.51901765
H	14.85837211	2.55161059	3.15239804
C	15.29666318	3.96929257	1.63298938
H	16.33410177	3.70236893	1.57944052
C	14.79102284	4.96941062	0.77475786
H	15.44853408	5.46500853	0.08687847
C	13.47799106	5.31076944	0.81485023

ELECTRONIC SUPPORTING INFORMATION

H	13.08778956	6.05186033	0.14090930
C	12.63844448	4.68633884	1.73696018
C	11.29399701	5.02631881	1.79841886
C	9.51276698	6.41468995	1.01731522
H	9.34270101	6.78792281	2.02185327
H	8.78535495	5.65390854	0.79504806
C	9.38500287	7.55173790	-0.01753300
H	8.39202824	7.97086216	0.02612625
H	9.56450157	7.14475418	-1.00628577
H	10.11255862	8.32587996	0.18729803
Sn	14.74830803	-3.85326048	3.57581843
S	12.89442639	-5.28672676	3.12729854
S	16.54033151	-4.35566720	2.09337704
O	11.95928461	-2.24908342	6.96306729
O	18.29117650	-0.89815011	5.03698377
N	19.39540023	-5.53070191	0.47964555
N	17.59029297	-2.50088133	3.63821815
N	9.77791267	-6.84929214	2.81253679
N	12.25084074	-3.62144728	5.18002679
C	15.44558644	-4.28467687	5.63618903
H	16.10487851	-3.51090294	6.00179857
H	14.59621137	-4.37740542	6.30671644
C	16.31241441	-5.61376237	5.55122550
H	15.75522297	-6.40406095	5.07330604
H	17.19808911	-5.38774958	4.96295830
C	16.74457761	-6.09634201	6.96458711
H	15.86029526	-6.39011413	7.51704599
H	17.24283037	-5.29460767	7.49507709
C	17.72406563	-7.29359276	6.85123777
H	17.98566818	-7.64253444	7.83879701
H	18.62284491	-6.98176243	6.32815167
H	17.25974985	-8.10297193	6.29630342
C	14.12257538	-1.73194952	3.29703037
H	13.03478090	-1.62844992	3.49269375
H	14.67966278	-1.11895289	3.95910241
C	14.55020040	-1.21378716	1.84525312
H	15.62619480	-1.35343552	1.77931047
H	14.31007108	-0.16244565	1.75381934
C	13.89445596	-1.93653114	0.67952864
H	12.83424001	-1.76087608	0.71396497
H	14.09489376	-2.98681183	0.73486031
C	14.48009089	-1.35164230	-0.62975230
H	14.00954891	-1.83440090	-1.47433962
H	15.55234213	-1.53874881	-0.66874804
H	14.30641881	-0.28687534	-0.67673576
C	17.85285340	-3.40859043	2.68027232
C	19.06215087	-3.64750413	2.18324928
C	19.29037054	-4.67718304	1.24681773
C	20.06989787	-2.83892236	2.59557828
C	21.35247336	-2.98114062	2.07957186
H	21.57319253	-3.73251529	1.33362498
C	22.32581915	-2.12748947	2.50553851

ELECTRONIC SUPPORTING INFORMATION

H	23.31932672	-2.20155053	2.10331424
C	22.04355936	-1.14029625	3.47378223
H	22.81641425	-0.46961419	3.79692189
C	20.79833698	-1.02995611	4.00404278
H	20.58456879	-0.27797816	4.74151051
C	19.79587311	-1.88546905	3.57370687
C	18.51972563	-1.76498792	4.09852596
C	16.96819484	-0.59066436	5.48997031
H	17.00071924	-0.31622333	6.52965988
H	16.31083181	-1.44234247	5.36506538
C	16.44766775	0.59827540	4.64820316
H	15.46024657	0.87667841	4.98228843
H	16.40901712	0.31337592	3.60483879
H	17.11982231	1.43894050	4.76645254
C	11.78389415	-4.57723797	4.32378728
C	10.51771287	-4.98761597	4.37334082
C	10.11103251	-6.01117396	3.51517987
C	9.64977725	-4.39752068	5.28446375
C	8.30695234	-4.77449167	5.36320240
H	7.92576748	-5.55673684	4.72977681
C	7.48747268	-4.13905579	6.24918602
H	6.45003803	-4.40598092	6.30273238
C	7.99311724	-3.13893911	7.10741520
H	7.33560586	-2.64334147	7.79529455
C	9.30615682	-2.79757554	7.06732352
H	9.69635058	-2.05648938	7.74126372
C	10.14568802	-3.42202514	6.14520255
C	11.49015515	-3.08203153	6.08374815
C	13.27137293	-1.69366000	6.86485788
H	13.44143890	-1.32042717	5.86031974
H	13.99878503	-2.45444139	7.08712497
C	13.39913695	-0.55661209	7.89970601
H	14.39211161	-0.13748769	7.85604677
H	13.21963827	-0.96359584	8.88845877
H	12.67158108	0.21752989	7.69487496

Optimized coordinates of the Dimer of Sn-Et held by N $\cdots$ H and C $\cdots$ H interactions

Sn	8.03645577	4.26115337	4.30297958
S	9.88451738	2.83400539	4.75585728
S	6.25337370	3.75646145	5.79466348
O	10.82047201	5.85780122	0.91907416
O	4.49202733	7.20945332	2.83997560
N	3.37897448	2.58297338	7.40006119
N	5.19489420	5.60932333	4.25303828
N	13.00318654	1.26076143	5.07559058
N	10.53367189	4.48141073	2.70583748
C	7.33635367	3.81880725	2.25406973
H	6.68643637	4.59568262	1.88924628
H	8.18164450	3.73242636	1.58866256
C	6.47671808	2.49610035	2.32944074
H	7.03453531	1.71096955	2.79950941
H	5.59676467	2.71417445	2.91668783

ELECTRONIC SUPPORTING INFORMATION

C	6.04222962	2.01668875	0.91438813
H	6.91742063	1.72220894	0.36640951
H	5.54399563	2.81155886	0.39365751
C	5.06134234	0.81251369	1.03381139
H	4.79886672	0.46828117	0.05022803
H	4.17078483	1.12453695	1.55160205
H	5.52593505	0.01251744	1.57918750
C	8.64811593	6.37472983	4.58628899
H	9.71747212	6.47962251	4.38090195
H	8.09543048	6.98752918	3.92041517
C	8.23594765	6.89095428	6.02964795
H	7.16922779	6.75595361	6.10835014
H	8.47919345	7.93657489	6.11798780
C	8.89570472	6.17164599	7.19929171
H	9.94977964	6.33809695	7.16862762
H	8.69335403	5.12346544	7.14727061
C	8.30424519	6.75188619	8.51598966
H	8.77154380	6.27708690	9.35392451
H	7.24212830	6.57075754	8.54820743
H	8.48095163	7.81218342	8.55806035
C	4.93077205	4.69089378	5.19651061
C	3.71504636	4.46106650	5.69692525
C	3.51387798	3.43016749	6.63632507
C	2.69674794	5.26964316	5.27775487
C	1.42273943	5.13767477	5.80425195
H	1.21385100	4.37808808	6.54216230
C	0.45494426	5.98283073	5.37736739
H	-0.53331965	5.90323276	5.77748673
C	0.74018372	6.96905917	4.40909537
H	-0.03347971	7.63481868	4.08367655
C	1.98277227	7.08278726	3.88189260
H	2.19529755	7.82511593	3.13826671
C	2.98024854	6.23223453	4.31459947
C	4.26389147	6.34787275	3.78858997
C	5.81515121	7.52040084	2.39373364
H	5.78599277	7.79118901	1.35749253
H	6.46512102	6.67094089	2.51832478
C	6.33718936	8.70750411	3.23358899
H	7.31941311	8.98223436	2.90252284
H	6.37575232	8.42446835	4.26982021
H	5.67229099	9.54303768	3.11618862
C	10.99710265	3.53001887	3.56058711
C	12.26743568	3.11789013	3.50991579
C	12.68864305	2.09611178	4.36269381
C	13.13751562	3.70925168	2.59347923
C	14.48024482	3.33626083	2.51734747
H	14.85849598	2.55754753	3.15323781
C	15.29757009	3.96759726	1.63099694
H	16.33261389	3.70214678	1.58123717
C	14.79187172	4.96878624	0.77520325
H	15.44810836	5.46346947	0.08717576
C	13.48065661	5.30857974	0.81533004

ELECTRONIC SUPPORTING INFORMATION

H	13.09037653	6.05188879	0.14465806
C	12.64107960	4.68324202	1.73623204
C	11.29481200	5.02013901	1.79812571
C	9.51136596	6.41257858	1.01658516
H	9.34340561	6.78327460	2.01361262
H	8.78682321	5.65751659	0.79389941
C	9.38460730	7.55332087	-0.01757395
H	8.39835070	7.97075268	0.02716303
H	9.56156478	7.15243779	-1.00013993
H	10.10721638	8.31991219	0.18943885
Sn	10.25876136	3.84720628	-3.57920457
S	12.10716269	5.27419245	-3.12659919
S	8.47564346	4.35189554	-2.08750849
O	13.04272548	2.25054958	-6.96309276
O	6.71428768	0.89889655	-5.04219738
N	5.60123640	5.52537511	-0.48210996
N	7.41715487	2.49902731	-3.62913472
N	15.23208445	6.84770288	-2.80980602
N	12.75614948	3.62683486	-5.17649915
C	9.55861459	4.28954493	-5.62810256
H	8.90869499	3.51266803	-5.99292469
H	10.40390360	4.37592272	-6.29351176
C	8.69897839	5.61224999	-5.55273205
H	9.25679536	6.39738055	-5.08266363
H	7.81902478	5.39417557	-4.96548513
C	8.26448973	6.09166127	-6.96778485
H	9.13968081	6.38614119	-7.51576339
H	7.76625585	5.29679120	-7.48851557
C	7.28360239	7.29583625	-6.84836164
H	7.02112681	7.64006877	-7.83194500
H	6.39304490	6.98381289	-6.33057103
H	7.74819499	8.09583255	-6.30298549
C	10.87037631	1.73362069	-3.29588296
H	11.93973177	1.62872579	-3.50127170
H	10.31768848	1.12082159	-3.96175665
C	10.45820768	1.21739606	-1.85252480
H	9.39148781	1.35239652	-1.77382279
H	10.70145335	0.17177511	-1.76418525
C	11.11796476	1.93670398	-0.68288126
H	12.17203964	1.77025304	-0.71354538
H	10.91561404	2.98488455	-0.73490238
C	10.52650520	1.35646380	0.63381666
H	10.99380380	1.83126310	1.47175151
H	9.46438830	1.53759246	0.66603443
H	10.70321162	0.29616658	0.67588735
C	7.15303190	3.41745663	-2.68566160
C	5.93730255	3.64728020	-2.18524485
C	5.73613880	4.67818664	-1.24585235
C	4.91900738	2.83870592	-2.60441814
C	3.64499996	2.97067497	-2.07792141
H	3.43611141	3.73026194	-1.34001076
C	2.67720458	2.12551939	-2.50480572

ELECTRONIC SUPPORTING INFORMATION

H	1.68894057	2.20511741	-2.10468615
C	2.96244381	1.13929092	-3.47307760
H	2.18878029	0.47353140	-3.79849639
C	4.20503247	1.02556279	-4.00028054
H	4.41755750	0.28323400	-4.74390628
C	5.20250920	1.87611539	-3.56757386
C	6.48615197	1.76047736	-4.09358323
C	8.03741163	0.58794917	-5.48843926
H	8.00825332	0.31716108	-6.52468041
H	8.68738134	1.43740921	-5.36384803
C	8.55944984	-0.59915409	-4.64858394
H	9.54167366	-0.87388418	-4.97964997
H	8.59801262	-0.31611843	-3.61235268
H	7.89455158	-1.43468773	-4.76598450
C	13.22007303	4.57777149	-4.32237477
C	14.48873462	4.99088572	-4.37227808
C	14.90196160	6.01193600	-3.51484023
C	15.36086731	4.39952533	-5.28866913
C	16.70287344	4.77215661	-5.36490002
H	17.08082037	5.55079892	-4.72896003
C	17.51990395	4.14075747	-6.25120031
H	18.55488659	4.40619302	-6.30094672
C	17.01413046	3.13955415	-7.10697833
H	17.67036705	2.64487783	-7.79499766
C	15.70291676	2.79975567	-7.06686319
H	15.31262070	2.05645441	-7.73751125
C	14.86363911	3.42520808	-6.14596528
C	13.51708642	3.08821916	-6.08404432
C	11.73362555	1.69577087	-6.86558781
H	11.56566547	1.32507509	-5.86856066
H	11.00908325	2.45083313	-7.08827407
C	11.60686761	0.55502905	-7.89974712
H	10.62061091	0.13759719	-7.85501001
H	11.78382495	0.95591220	-8.88231296
H	12.32947665	-0.21156214	-7.69273416