SUPPORTING INFORMATION (II) FOR

13-Methyl-2,6-dithia[7]metacyclophane - A useful molecule to connect VT NMR results and structure with calculations

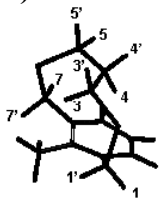
Reginald H. Mitchell,[*†] Rachel Blunden,[†] Gavin Hollett,[†] Subhajit Bandyopadhyay,[†]
Richard Vaughan Williams[*‡] and Brendan Twamley[‡]

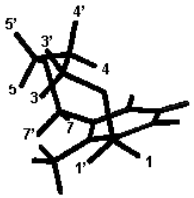
Contribution from (†) the Department of Chemistry, University of Victoria, PO Box 3065, Victoria, BC, Canada, V8W 3V6 and (‡) the Department of Chemistry, University of Idaho, PO Box 442343, Moscow, Idaho 83844-2343.

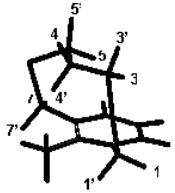
REGINALD MITCHELL
PHONE: 250-721-7159
FAX: 250-721-7147
E-MAIL: REGMITCH@UVIC.CA

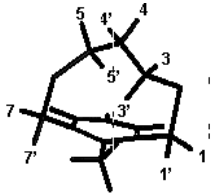
CONTENTS

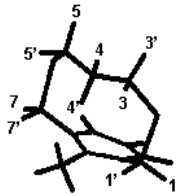
Table S1. Experimental (175K) and calculated (1a - 1f) chemical shifts (δ) for the protons and carbons of 1, and differences (Δ) between experimental and calculated values, or differences (Δ') between experimental or calculated values for analogous atoms (ppm).[a]

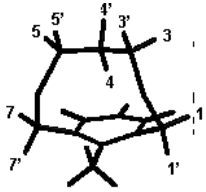

1a


1b


1c


1d


1e


1f

#	175K	1a	1b	1c	1d	1e	1f	Δ(1a)	Δ(1b)	Δ(1c)	Δ(1d)	Δ(1e)	Δ(1f)
Hydrogens													
1	3.53	3.14	3.18	3.54	2.99	3.44	3.26	0.39	0.35	-0.01	0.54	0.09	0.27
1'	4.35	3.94	3.83	3.82	3.83	3.91	3.62	0.41	0.52	0.53	0.52	0.43	0.73
Δ'(1'-1)	0.82	0.80	0.65	0.28	0.84	0.47	0.36						
7	3.87	3.47	3.18	3.54	3.45	3.24	3.26	0.40	0.59	0.33	0.42	0.63	0.63
7'	3.71	3.45	3.83	3.82	3.65	3.61	3.62	0.26	-0.12	-0.11	0.06	0.10	0.10
Δ'(7'-7)	-0.16	-0.02	0.65	0.28	0.20	0.37	0.36						
3	2.39	2.06	1.81	0.18	2.36	0.14	2.08	0.33	0.58	2.21	0.03	2.25	0.21
3'	2.05	1.60	1.99	1.65	2.07	1.28	1.52	0.45	0.06	0.40	-0.02	0.77	0.53
Δ'(3'-3)	0.34	0.46	0.18	1.47	-0.29	1.14	-0.56						
5	2.05	1.46	1.81	0.19	-0.24	1.59	2.08	0.59	0.24	1.86	2.29	0.46	0.46
5'	2.61	2.14	1.99	1.65	1.84	2.61	1.52	0.47	0.62	0.96	0.77	0.00	1.09
Δ'(5'-5)	0.56	0.68	0.18	1.46	2.08	1.02	-0.56						
4	-1.79	-1.92	-0.87	1.61	1.13	1.47	-2.08	0.13	-0.92	-3.40	2.92	-3.26	0.29
4'	1.06	0.71	1.25	0.86	1.00	1.28	0.47	0.35	-0.19	0.20	0.06	-0.22	0.59
Δ'(4'-4)	2.85	2.63	2.12	-0.75	-0.13	-0.19	2.55						
9	6.94	7.14	7.48	7.28	7.09	7.46	7.10	-0.20	-0.54	-0.34	-0.15	-0.52	-0.16
10	6.94	7.26	7.44	7.32	7.32	7.42	7.06	-0.32	-0.50	-0.38	-0.38	-0.48	-0.12
11	7.12	7.48	7.48	7.29	7.42	7.26	7.10	-0.36	-0.36	-0.17	-0.30	-0.14	0.02

							S(II)4						
14		3.26	2.37	2.77	3.40	1.97	2.16						
14'		2.24	2.19	2.04	2.26	2.15	2.16						
14"		2.09	2.19	2.76	2.09	2.60	4.18						
14av	2.49	2.53	2.25	2.52	2.58	2.24	2.84	-0.04	0.24	-0.03	-0.09	0.25	-0.35
Carbons													
1	34.08	40.63	41.99	40.86	41.88	41.31	44.42	-6.55	-7.91	-6.78	-7.80	-7.23	-10.32
7	35.86	42.61	41.99	40.92	42.41	39.42	44.42	-6.75	-6.13	-5.06	-6.55	-3.56	-8.56
Δ'(7-1)	1.78	1.98	0.00	0.06	0.53	-1.89	0.00						
3	25.56	32.47	38.68	34.54	32.09	31.82	36.81	-6.91	-13.12	-8.97	-6.53	-6.26	-11.25
5	30.04	36.45	38.68	34.52	30.32	37.54	36.81	-6.41	-8.64	-4.48	-0.28	-7.50	-6.77
Δ'(5-3)	4.48	3.98	0.00	-0.02	-1.77	5.72	0.00						
4	29.23	32.12	36.21	39.22	32.73	32.27	27.02	-2.89	-6.98	-9.98	-3.50	-3.04	2.21
14	18.41	18.55	19.03	16.75	17.62	17.96	20.02	-0.14	-0.62	1.66	0.79	0.45	-1.61
8	138.21	141.26	143.29	137.93	140.14	144.74	143.23	-3.05	-5.08	0.28	-1.93	-6.53	-5.02
12	138.13	142.17	143.29	137.93	145.53	136.77	143.23	-4.04	-5.16	0.20	-7.40	1.36	-5.10
Δ'(12-8)	-0.08	0.91	0.00	0.00	5.39	-7.97	0.00						
9	126.35	128.55	130.50	133.21	130.34	131.02	128.10	-2.20	-2.65	-6.86	-3.99	-4.67	-1.75
11	127.85	131.37	130.50	133.22	130.04	129.46	128.10	-3.52	-2.65	-5.37	-2.19	-1.61	-0.25
Δ'(11-9)	1.50	2.82	0.00	0.01	-0.20	-1.56	0.00						
10	126.19	127.36	128.79	126.27	126.79	128.19	124.97	-1.17	-2.60	-0.08	-0.60	-2.00	1.22
13	136.74	141.63	138.57	141.76	138.20	136.77	150.30	-4.89	-1.83	-5.02	-1.46	-0.03	-13.56

[a] assignments of the carbons were made on the basis of HMBC and HMQC experiments, and on which signals collapse under VT conditions.

Table S2. Relative energies for the conformers 1a-f (kcal/mol)**.**

Conformer	E_{DFT}	E_{RHF}	E_{MM}	E_{PCM}	E_{AM1}
1a	0	0	0	0	0
1b	0.795	0.78	-1.01	-2.11	-1.24
1c	1.060	1.17	2.81	-1.96	-1.31
1d	1.753	2.54	2.64	3.78	1.31
1e	4.954	6.18	6.44	8.28	3.30
1f	8.451	10.24	13.12	10.76	8.18

E_{DFT} = DFT B3LYP/6-31G* (including zero-point correction) (see text)[1]
E_{RHF} = RHF 6-31G* (Spartan)[2]
E_{MM} = MMFF (Spartan) Molecular Mechanics[2]
E_{PCM} = PCMODEL MMX (Molecular Mechanics + pi)[3]
E_{AM1} = AM1 (Spartan)[2]

Note: Second derivative (frequency) calculations to verify true minima were only performed for the B3LYP/6-31G* method. The incomplete electron correlation incorporated in the standard parameterization of the semiempirical methods is known to lead to erroneous geometries and energies in aromatic systems.[4] Although geometries are similar by inspection, they are not identical by the various methods, and when single point energies using MM and AM1 are run on the DFT minimized geometries, quite different energies are obtained. The data is thus presented only for comparison of the values obtained. For comparisons in related cyclophanes see reference 5.

1) See text, reference 9.
2) Spartan 02 v 1.0.1, Wavefunction Inc, Irvine, CA, 92612, USA.
3) PCMODEL v 8.0, Serena Software, Box 3076, Bloomington, IN 47402-3076, USA.
4) Williams, R. V.; Edwards, W. D.; Vij, A.; Tolbert, R. W.; Mitchell, R. H. *J. Org. Chem*., **1998**, *63*, 3125-3127.
5) Mitchell. R. H. *J. Am. Chem. Soc*. **2002**, *124*, 2352-2357

Table S3: Cartesian Coordinates for **1a-f**, **1*** and **2a**

1a

1	6	0	-1.508789	1.890712	-0.734729
2	6	0	-1.329056	1.101563	0.413390
3	6	0	-0.043439	0.965000	0.973781
4	6	0	-0.421961	2.464684	-1.383059
5	6	0	0.866752	2.135619	-0.958291
6	6	0	1.064730	1.360600	0.188458
7	6	0	-2.459007	0.214596	0.864002
8	16	0	-2.520177	-1.370520	-0.140338
9	6	0	-0.760130	-1.944842	-0.190904
10	6	0	0.083861	-1.359874	-1.336781
11	6	0	1.613149	-1.553469	-1.223502
12	16	0	2.503147	-1.075106	0.329134
13	6	0	2.434469	0.789298	0.451543
14	6	0	0.176640	0.377859	2.354395
15	1	0	-0.569601	3.092856	-2.257154
16	1	0	-2.510833	2.012190	-1.138880
17	1	0	1.729137	2.458542	-1.537029
18	1	0	-3.437287	0.666514	0.673850
19	1	0	-2.409038	-0.051120	1.920504
20	1	0	-0.839504	-3.033770	-0.285430
21	1	0	-0.301311	-1.751842	0.778803
22	1	0	-0.138343	-0.301566	-1.459999
23	1	0	-0.221066	-1.838884	-2.277871
24	1	0	2.098261	-1.062719	-2.074333
25	1	0	1.868153	-2.618513	-1.288496
26	1	0	2.795599	0.968400	1.470684
27	1	0	3.166432	1.217282	-0.239250
28	1	0	0.512678	-0.663698	2.340756
29	1	0	0.953335	0.946811	2.878538
30	1	0	-0.727435	0.439055	2.964745

1b

1	6	0	-2.072351	-0.756633	1.199112
2	6	0	-1.220201	0.354818	1.211710
3	6	0	-0.898305	1.006706	0.000000
4	6	0	-2.549274	-1.277855	0.000000
5	6	0	-2.072351	-0.756633	-1.199112
6	6	0	-1.220201	0.354818	-1.211710
7	6	0	-0.492770	0.682575	2.492457
8	16	0	0.968616	-0.447110	2.778855
9	6	0	2.023173	-0.163274	1.288103

10	6	0	1.638187	-0.935599	0.000000
11	6	0	2.023173	-0.163274	-1.288103
12	6	0	-0.492770	0.682575	-2.492457
13	6	0	-0.216496	2.365094	0.000000
14	1	0	-3.229347	-2.125145	0.000000
15	1	0	-2.327973	-1.236659	2.140655
16	1	0	-2.327973	-1.236659	-2.140655
17	1	0	-1.118166	0.498824	3.371940
18	1	0	-0.143403	1.715410	2.543590
19	1	0	3.028760	-0.439053	1.622952
20	1	0	2.050346	0.916130	1.110539
21	1	0	0.571334	-1.144959	0.000000
22	1	0	2.134386	-1.912904	0.000000
23	1	0	3.028760	-0.439053	-1.622952
24	1	0	2.050346	0.916130	-1.110539
25	1	0	-0.143403	1.715410	-2.543590
26	1	0	-1.118166	0.498824	-3.371940
27	1	0	0.878768	2.327500	0.000000
28	1	0	-0.514436	2.946916	-0.876902
29	1	0	-0.514436	2.946916	0.876902
30	16	0	0.968616	-0.447110	-2.778855

1c

1	6	0	-1.203543	2.105622	-0.732890
2	6	0	-1.214265	1.204870	0.341908
3	6	0	0.000649	0.818167	0.947811
4	6	0	-0.005027	2.593364	-1.246922
5	6	0	1.196337	2.108157	-0.737019
6	6	0	1.212650	1.207461	0.337693
7	6	0	-2.519013	0.555021	0.712284
8	1	0	-1.114765	-0.465088	-1.624067
9	6	0	-1.297858	-1.427183	-1.138941
10	6	0	1.300695	-1.429050	-1.138815
11	6	0	2.520320	0.561260	0.704469
12	6	0	0.004277	-0.002047	2.221526
13	1	0	-0.007184	3.304874	-2.067953
14	1	0	-2.148403	2.406687	-1.178982
15	1	0	2.139000	2.411370	-1.186289
16	1	0	-2.657277	0.461169	1.791586
17	1	0	-1.700259	-2.094456	-1.907580
18	16	0	-2.712477	-1.202173	0.035241
19	1	0	1.704644	-2.099019	-1.904263
20	6	0	0.000896	-2.001983	-0.518385
21	1	0	2.664535	0.473434	1.783578

22	1	0	3.354487	1.138282	0.299145
23	1	0	0.882789	-0.646215	2.297852
24	1	0	0.007771	0.665325	3.095062
25	1	0	-0.874466	-0.645078	2.304010
26	16	0	2.713077	-1.199581	0.037344
27	1	0	0.000926	-1.815118	0.552536
28	1	0	-0.000006	-3.094068	-0.619065
29	1	0	1.118243	-0.468727	-1.627720
30	1	0	-3.356335	1.132725	0.314491

1d

1	6	0	-0.959089	2.268000	-0.740038
2	6	0	-0.983407	1.422616	0.383636
3	6	0	0.227079	1.005091	0.965913
4	6	0	0.239718	2.622147	-1.343351
5	6	0	1.419421	2.015782	-0.903659
6	6	0	1.415634	1.184435	0.218527
7	6	0	-2.295207	0.789030	0.766273
8	16	0	-2.636952	-0.716358	-0.286713
9	6	0	-1.330077	-1.948385	0.193387
10	6	0	0.839034	-1.456597	-1.234886
11	6	0	2.587989	0.276915	0.460630
12	6	0	0.306114	0.347048	2.329837
13	1	0	0.250555	3.293437	-2.197510
14	1	0	-1.901375	2.610850	-1.160661
15	1	0	2.344209	2.156330	-1.458424
16	1	0	-3.142783	1.441886	0.535557
17	1	0	-2.372335	0.509524	1.817627
18	1	0	-1.885082	-2.830781	0.526125
19	1	0	-0.789116	-1.571353	1.060904
20	1	0	1.293823	-1.775364	-2.177515
21	6	0	-0.354807	-2.375693	-0.920943
22	1	0	2.906459	0.234224	1.506348
23	1	0	3.445674	0.576005	-0.146321
24	1	0	0.716301	-0.667284	2.290086
25	1	0	0.972468	0.934415	2.974994
26	1	0	-0.661900	0.304777	2.831889
27	16	0	2.169809	-1.521969	0.062509
28	1	0	0.027267	-3.370773	-0.653700
29	1	0	-0.917855	-2.511931	-1.854017
30	1	0	0.513561	-0.423083	-1.360079

1e

1	6	0	-0.395909	2.613118	-1.219177

2	6	0	-1.545663	1.923968	-0.830723
3	6	0	-1.515375	1.051576	0.260147
4	6	0	-0.329540	0.903475	1.019141
5	6	0	0.868134	1.401025	0.470950
6	6	0	0.811428	2.298922	-0.608622
7	6	0	-2.648041	0.089754	0.460551
8	16	0	-2.340155	-1.553266	-0.443160
9	6	0	-0.556874	-1.565786	-0.956243
10	6	0	0.409325	-2.137225	0.091730
11	6	0	1.919991	-2.028712	-0.193684
12	16	0	2.730477	-0.397619	-0.535312
13	6	0	2.215041	0.799540	0.804339
14	6	0	-0.387223	0.233769	2.379436
15	1	0	-0.429186	3.321297	-2.042393
16	1	0	-2.467494	2.035377	-1.396397
17	1	0	1.739269	2.706610	-1.002836
18	1	0	-2.835723	-0.148813	1.508027
19	1	0	-3.575199	0.467100	0.022560
20	1	0	-0.562805	-2.194752	-1.853755
21	1	0	-0.267733	-0.563366	-1.275416
22	1	0	0.196370	-3.208271	0.215006
23	1	0	0.208616	-1.692866	1.064131
24	1	0	2.455424	-2.508008	0.633490
25	1	0	2.179792	-2.585685	-1.102366
26	1	0	3.013312	1.547932	0.776429
27	1	0	2.267093	0.303982	1.774444
28	1	0	-0.903946	0.901782	3.081812
29	1	0	0.601620	0.043411	2.800379
30	1	0	-0.936347	-0.712131	2.385382

1f

1	6	0	-2.627780	-1.276918	0.000000
2	6	0	-2.124761	-0.773409	1.199572
3	6	0	-1.265897	0.334473	1.204001
4	6	0	-0.990499	1.012136	0.000000
5	6	0	-1.265897	0.334473	-1.204001
6	6	0	-2.124761	-0.773409	-1.199572
7	6	0	-0.425961	0.625411	2.423420
8	16	0	1.401745	0.449014	2.073306
9	6	0	1.643910	-1.238474	1.355136
10	6	0	1.058060	-1.697651	0.000000
11	6	0	1.643910	-1.238474	-1.355136
12	16	0	1.401745	0.449014	-2.073306
13	6	0	-0.425961	0.625411	-2.423420

14	6	0	-0.309755	2.361680	0.000000
15	1	0	-3.316312	-2.117459	0.000000
16	1	0	-2.362403	-1.266201	2.139799
17	1	0	-2.362403	-1.266201	-2.139799
18	1	0	-0.496899	1.660036	2.777688
19	1	0	-0.706441	-0.029455	3.254117
20	1	0	2.739100	-1.303528	1.327180
21	1	0	1.312258	-1.960474	2.110017
22	1	0	-0.024763	-1.601309	0.000000
23	1	0	1.242744	-2.784588	0.000000
24	1	0	2.739100	-1.303528	-1.327180
25	1	0	1.312258	-1.960474	-2.110017
26	1	0	-0.706441	-0.029455	-3.254117
27	1	0	-0.496899	1.660036	-2.777688
28	1	0	-0.608138	2.938743	0.881837
29	1	0	-0.608138	2.938743	-0.881837
30	1	0	0.779881	2.285178	0.000000

1*

1	6	0	-1.468680	1.917682	-0.820597
2	6	0	-1.383640	1.121401	0.332661
3	6	0	-0.133152	0.927270	0.954765
4	6	0	-0.331158	2.464891	-1.402899
5	6	0	0.919937	2.130094	-0.887243
6	6	0	1.025996	1.344435	0.264514
7	6	0	-2.588283	0.305079	0.716436
8	16	0	-2.624150	-1.315405	-0.219777
9	6	0	-0.896705	-1.949757	-0.059632
10	6	0	0.105921	-1.484542	-1.134281
11	6	0	1.560742	-1.911845	-0.831926
12	16	0	2.890462	-0.853560	-0.002120
13	6	0	2.370575	0.831564	0.683072
14	6	0	0.018006	0.266528	2.312944
15	1	0	-0.413036	3.094631	-2.284423
16	1	0	-2.441403	2.072020	-1.281212
17	1	0	1.825480	2.455978	-1.393093
18	1	0	-3.517925	0.794346	0.411402
19	1	0	-2.660391	0.094657	1.784077
20	1	0	-1.013844	-3.037782	-0.122406
21	1	0	-0.537754	-1.743013	0.948550
22	1	0	0.032234	-0.415775	-1.321788
23	1	0	-0.174138	-1.970305	-2.077971
24	1	0	2.055421	-2.146373	-1.777678
25	1	0	1.551479	-2.831504	-0.237430

26	1	0	2.465031	0.755362	1.766975
27	1	0	3.165459	1.486292	0.317629
28	1	0	0.703499	-0.587819	2.295429
29	1	0	0.431754	0.986889	3.031050
30	1	0	-0.930209	-0.080955	2.724356

2a

1	6	0	1.249286	1.064832	0.569830
2	6	0	-0.041616	1.145433	1.106694
3	6	0	-0.735552	-0.029741	1.454751
4	6	0	1.862446	-0.158218	0.274763
5	6	0	1.061791	-1.300101	0.410616
6	6	0	-0.227665	-1.245569	0.954604
7	6	0	-0.767661	2.463714	1.062457
8	16	0	-1.504628	2.780015	-0.634924
9	6	0	-2.332722	1.185451	-1.084979
10	6	0	-1.425245	0.135382	-1.749883
11	6	0	-1.991180	-1.300965	-1.815757
12	16	0	-2.616636	-2.122622	-0.278377
13	6	0	-1.125544	-2.447397	0.798598
14	6	0	-1.999208	0.005760	2.292124
15	6	0	3.309254	-0.200881	-0.248017
16	6	0	4.246937	0.421248	0.813971
17	6	0	3.787413	-1.638316	-0.527499
18	6	0	3.418376	0.607457	-1.562537
19	1	0	1.761842	1.995934	0.341044
20	1	0	1.425281	-2.262829	0.066116
21	1	0	-0.092279	3.313885	1.199495
22	1	0	-1.564578	2.540706	1.803711
23	1	0	-3.133483	1.491625	-1.767760
24	1	0	-2.821627	0.779809	-0.199066
25	1	0	-0.453596	0.117479	-1.259770
26	1	0	-1.231463	0.442915	-2.787188
27	1	0	-1.250134	-1.955423	-2.287734
28	1	0	-2.885345	-1.330201	-2.450640
29	1	0	-1.583386	-2.780174	1.737207
30	1	0	-0.566441	-3.292872	0.387438
31	1	0	-2.920969	0.114118	1.711831
32	1	0	-2.101362	-0.920942	2.865485
33	1	0	-1.959514	0.825977	3.015669
34	1	0	5.284880	0.413068	0.459135
35	1	0	3.976751	1.459280	1.034438
36	1	0	4.204262	-0.141997	1.753244
37	1	0	4.828922	-1.620697	-0.867658

38	1	0	3.741784	-2.264659	0.370679
39	1	0	3.194526	-2.121396	-1.312700
40	1	0	4.448832	0.586236	-1.938227
41	1	0	2.766004	0.187170	-2.336480
42	1	0	3.136666	1.656172	-1.423866

Table S4: Total B3LYP/6-31G* energies, zero-point corrections, free energies and enthalpies (Hartrees) for the conformers **1a**-**1f** and **1***

Molecule	Total E	Zero-point correction	E+ZPE	Thermal	Enthalpy	Free Energy
1a	-1263.27970218	0.254233	-1263.025469	-1263.012060	-1263.011116	-1263.064
1b	-1263.27820205	0.254000	-1263.024202	-1263.010556	-1263.009612	-1263.064
1c	-1263.27824546	0.254467	-1263.023779	-1263.010181	-1263.009237	-1263.063
1d	-1263.27669717	0.254021	-1263.022676	-1263.009165	-1263.008221	-1263.061
1e	-1263.27168972	0.254115	-1263.017575	-1263.004009	-1263.003065	-1263.057
1f	-1263.26569857	0.253696	-1263.012002	-1262.998594	-1262.997649	-1263.050
1*	-1263.26628388	0.254535	-1263.011749	-1262.999005	-1262.998061	-1263.050

Table S5. Crystal data and structure refinement for 1.

	1
Empirical formula	$C_{12}H_{16}S_2$
Fw	224.37
λ (Å)	0.71073
Cryst syst; space group	Orthorhombic, Pbca
Color, habit	Colorless plate
Crystal dim, mm	0.29, 0.22, 0.04
T/°C	85(2)
a (Å)	12.260(3)
b (Å)	7.9032(16)
c (Å)	23.177(5)
V (Å^3)	2245.7(9)
Z	8
D_{calc} (Mg m^{-3})	1.327
μ (mm^{-1})	0.432
Data/restraints/parameters	2032 / 18 / 128
Index ranges	$-14 \le h \le 14$, $-9 \le k \le 8$, $-27 \le l \le 25$
Goodness of Fit on F^2	1.087
Final R indices [I>2s(I)]	$R_1 = 0.0504$, $wR_2 = 0.1146$
R indices (all data)	$R_1 = 0.0794$, $wR_2 = 0.1291$

$R = \Sigma \mid F_o \mid - \mid F_c \mid / \Sigma \mid F_o \mid$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma [w(F_o^2)^2]\}^{1/2}$

Table S6. Atomic coordinates (x 10) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8000(3)	1039(5)	6736(2)	17(1)
C(3)	9652(3)	3578(4)	6943(2)	14(1)
C(4)	10755(2)	2728(4)	6843(1)	13(1)
C(5)	11507(3)	3627(5)	6410(2)	17(1)
C(7)	10831(3)	2293(4)	5296(2)	17(1)
C(8)	10247(3)	963(4)	5637(1)	13(1)
C(9)	10809(3)	-455(4)	5819(2)	15(1)
C(10)	10386(3)	-1548(4)	6227(2)	17(1)
C(11)	9429(3)	-1098(4)	6506(2)	14(1)
C(12)	8848(2)	336(4)	6333(1)	11(1)
C(13)	9191(3)	1266(4)	5859(1)	12(1)
C(14)	8473(3)	2630(5)	5594(2)	17(1)
S(2)	8646(1)	2276(1)	7317(1)	15(1)
S(6)	10977(1)	4255(1)	5704(1)	18(1)

Table S7. Bond lengths [Å] and angles [°] for 1.

C(1)-C(12)	1.504(5)	C(13)-C(14)	1.521(5)
C(1)-S(2)	1.843(4)	C(14)-H(14A)	0.9800
C(1)-H(1A)	0.9900	C(14)-H(14B)	0.9800
C(1)-H(1B)	0.9900	C(14)-H(14C)	0.9800
C(3)-C(4)	1.528(4)		
C(3)-S(2)	1.825(3)	C(12)-C(1)-S(2)	110.6(2)
C(3)-H(3A)	0.9900	C(12)-C(1)-H(1A)	109.5
C(3)-H(3B)	0.9900	S(2)-C(1)-H(1A)	109.5
C(4)-C(5)	1.537(5)	C(12)-C(1)-H(1B)	109.5
C(4)-H(4A)	0.9900	S(2)-C(1)-H(1B)	109.5
C(4)-H(4B)	0.9900	H(1A)-C(1)-H(1B)	108.1
C(5)-S(6)	1.829(4)	C(4)-C(3)-S(2)	114.9(2)
C(5)-H(5A)	0.9900	C(4)-C(3)-H(3A)	108.5
C(5)-H(5B)	0.9900	S(2)-C(3)-H(3A)	108.5
C(7)-C(8)	1.497(5)	C(4)-C(3)-H(3B)	108.5
C(7)-S(6)	1.825(4)	S(2)-C(3)-H(3B)	108.5
C(7)-H(7A)	0.9900	H(3A)-C(3)-H(3B)	107.5
C(7)-H(7B)	0.9900	C(3)-C(4)-C(5)	115.2(3)
C(8)-C(9)	1.381(5)	C(3)-C(4)-H(4A)	108.5
C(8)-C(13)	1.414(5)	C(5)-C(4)-H(4A)	108.5
C(9)-C(10)	1.383(5)	C(3)-C(4)-H(4B)	108.5
C(9)-H(9)	0.9500	C(5)-C(4)-H(4B)	108.5
C(10)-C(11)	1.385(5)	H(4A)-C(4)-H(4B)	107.5
C(10)-H(10)	0.9500	C(4)-C(5)-S(6)	119.7(2)
C(11)-C(12)	1.398(5)	C(4)-C(5)-H(5A)	107.4
C(11)-H(11)	0.9500	S(6)-C(5)-H(5A)	107.4
C(12)-C(13)	1.386(5)	C(4)-C(5)-H(5B)	107.4

S(6)-C(5)-H(5B)	107.4
H(5A)-C(5)-H(5B)	106.9
C(8)-C(7)-S(6)	111.7(2)
C(8)-C(7)-H(7A)	109.3
S(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7B)	109.3
S(6)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
C(9)-C(8)-C(13)	118.9(3)
C(9)-C(8)-C(7)	119.5(3)
C(13)-C(8)-C(7)	120.7(3)
C(8)-C(9)-C(10)	121.9(3)
C(8)-C(9)-H(9)	119.0
C(10)-C(9)-H(9)	119.0
C(9)-C(10)-C(11)	118.4(3)
C(9)-C(10)-H(10)	120.8
C(11)-C(10)-H(10)	120.8
C(10)-C(11)-C(12)	120.4(3)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(13)-C(12)-C(11)	120.2(3)
C(13)-C(12)-C(1)	120.3(3)
C(11)-C(12)-C(1)	118.3(3)
C(12)-C(13)-C(8)	118.4(3)
C(12)-C(13)-C(14)	121.4(3)
C(8)-C(13)-C(14)	120.2(3)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(3)-S(2)-C(1)	104.04(17)
C(7)-S(6)-C(5)	105.52(17)

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	6(2)	21(2)	24(2)	4(2)	0(1)	-1(1)
C(3)	9(2)	14(2)	20(2)	-1(2)	1(1)	0(1)
C(4)	9(2)	13(2)	16(2)	0(2)	-1(1)	-3(1)

C(5)	11(2)	18(2)	24(2)	-1(2)	-2(2)	-2(2)
C(7)	14(2)	17(2)	18(2)	0(2)	3(1)	0(2)
C(8)	11(2)	15(2)	14(2)	-1(2)	-2(1)	-2(1)
C(9)	9(2)	14(2)	21(2)	-6(2)	1(1)	0(1)
C(10)	18(2)	11(2)	22(2)	-3(2)	-6(2)	4(2)
C(11)	14(1)	14(1)	15(1)	0(1)	-1(1)	-3(1)
C(12)	9(1)	12(1)	13(1)	-1(1)	-1(1)	-2(1)
C(13)	10(1)	11(1)	13(1)	-2(1)	-2(1)	-1(1)
C(14)	11(2)	18(2)	22(2)	2(2)	-6(1)	2(2)
S(2)	8(1)	18(1)	20(1)	0(1)	3(1)	1(1)
S(6)	14(1)	16(1)	23(1)	3(1)	1(1)	-4(1)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	7574	99	6905	20
H(1B)	7491	1772	6517	20
H(3A)	9347	3915	6564	17
H(3B)	9770	4624	7170	17
H(4A)	10625	1560	6705	15
H(4B)	11140	2647	7218	15
H(5A)	12142	2878	6342	21
H(5B)	11788	4660	6601	21
H(7A)	10421	2522	4937	20
H(7B)	11562	1869	5188	20
H(9)	11506	-686	5658	18
H(10)	10742	-2584	6314	21
H(11)	9167	-1768	6816	17
H(14A)	7710	2262	5603	26

H(14B)	8697	2827	5194	26
H(14C)	8550	3681	5815	26

Table S10 An estimation of the deviation from planarity of the phenyl core moiety for 1a, 2 and X-ray results

	1a	**2**	**X-ray**
C8	0.1238	0.1192	0.1125
C9	-0.0042	0.0041	0.0048
C10	-0.1334	-0.1353	-0.1298
C11	0.0025	-0.0009	0.0001
C12	0.1200	0.1234	0.1172
C13	0.0256	0.0237	0.0217
C14	-0.1344	-0.1342	-0.1263
Mean deviation from plane (Å)			
	0.0777	0.0773	0.0732

Table S11 OFIT overlay comparison of the Phenyl core for 1a, 2 and X-ray results.

Atom Model deviation Å	**2/X-ray**	**1a/X-ray**	**1a/2**
C8	0.009	0.017	0.015
C9	0.006	0.017	0.007
C10	0.019	0.020	0.016
C11	0.003	0.014	0.029
C12	0.008	0.005	0.014
C13	0.012	0.015	0.018
C14	0.010	0.015	0.017
Deviation	**0.0107**	**0.0153**	**0.0175**