Australian Journal of Chemistry **2008**, *61*, 981–985. doi: 10.1071/CH08328

Why are Fluorene-Containing Materials so Versatile? An Electronic Structure Perspective

Igor Novak[A,C] *and Branka Kovač*[B,C]

[A]Charles Sturt University, POB 883, Orange, NSW 2800, Australia.

[B]Physical Chemistry Department, Ruđer Bošković Institute, HR-10002 Zagreb, Croatia.

[C]Corresponding authors. Email: inovak@csu.edu.au; bkovac@irb.hr

Accessory Publication: coordinates of optimized geometries, total energies and number of imaginary frequencies for substituted fluorenes.

(x,y,z, in Angstroms; absolute electron energies in a.u.)

9-trimethylsilylfluorene NIMAG=0

	x	y	z
c	0.245275	-2.317200	3.017003
c	-0.332683	-1.119077	3.464609
c	-0.728790	-0.129916	2.552058
c	-0.543174	-0.348760	1.184404
c	0.019675	-1.571064	0.733930
c	0.422036	-2.552144	1.648622
h	0.548512	-3.070007	3.737315
h	-0.478228	-0.957158	4.527803
h	-1.181234	0.788088	2.912564
h	0.854383	-3.486850	1.305044
c	-0.864172	0.546773	0.000000
h	-1.912571	0.874992	0.000000
c	-0.543174	-0.348760	-1.184404
c	-0.728790	-0.129916	-2.552058
c	-0.332683	-1.119077	-3.464609
c	0.245275	-2.317200	-3.017003
c	0.422036	-2.552144	-1.648622
c	0.019675	-1.571064	-0.733930
h	-1.181234	0.788088	-2.912564
h	-0.478228	-0.957158	-4.527803
h	0.548512	-3.070007	-3.737315
h	0.854383	-3.486850	-1.305044
si	0.217283	2.195656	0.000000
c	-0.207699	3.241260	1.553616
h	0.121887	2.746996	2.472630
h	0.297112	4.212787	1.493762
h	-1.285261	3.427994	1.628115
c	-0.207699	3.241260	-1.553616
h	0.121887	2.746996	-2.472630

h	-1.285261	3.427994	-1.628115
h	0.297112	4.212787	-1.493762
c	2.074913	1.735207	0.000000
h	2.331683	1.146152	-0.886477
h	2.692781	2.640767	0.000000
h	2.331683	1.146152	0.886477

total energy = -105.3790157

2-aminofluorene NIMAG=0

	x	y	z
h	0.339375	-2.465057	-0.881132
c	-2.571649	1.327212	-0.000001
c	-3.072206	0.004053	-0.000004
c	-2.161590	-1.078904	-0.000001
c	-0.796472	-0.821485	0.000006
c	-0.298841	0.504236	0.000008
c	-1.197929	1.576898	0.000004
h	-3.272047	2.157686	-0.000004
h	-2.538649	-2.098642	-0.000003
h	-0.840788	2.602311	0.000006
c	0.361422	-1.810275	0.000010
h	0.339378	-2.465037	0.881169
c	1.580826	-0.898183	0.000003
c	2.933225	-1.229461	-0.000007
c	3.889298	-0.199567	-0.000011
c	3.485487	1.143194	-0.000004
c	2.125540	1.482846	0.000004
c	1.170576	0.458846	0.000006
h	3.251685	-2.268100	-0.000012
h	4.946368	-0.444929	-0.000019
h	4.234630	1.928713	-0.000005
h	1.822907	2.525532	0.000008
n	-4.438922	-0.228408	-0.000009
h	-4.803790	-1.164474	-0.000009
h	-5.092750	0.534387	-0.000018

total energy = -90.2036044

2,7-dibromofluorene NIMAG=0

	x	y	z
h	0.000000	-2.273517	0.880818
c	3.018936	1.431525	0.000034
c	3.444078	0.101168	-0.000033
c	2.540126	-0.963859	0.000014

c	1.182671	-0.668311	0.000129
c	0.733708	0.668788	0.000170
c	1.653408	1.719491	0.000129
h	3.751209	2.231275	0.000011
h	2.901832	-1.986987	-0.000041
h	1.322458	2.754563	0.000177
c	0.000000	-1.616396	0.000447
h	0.000000	-2.274617	-0.879077
c	-1.182671	-0.668311	0.000129
c	-2.540126	-0.963859	0.000014
c	-3.444078	0.101168	-0.000033
c	-3.018936	1.431525	0.000034
c	-1.653408	1.719491	0.000129
c	-0.733708	0.668788	0.000170
h	-2.901832	-1.986987	-0.000041
h	-3.751209	2.231275	0.000011
h	-1.322458	2.754563	0.000177
br	5.320178	-0.274526	-0.000143
br	-5.320178	-0.274526	-0.000143

total energy = -5643.6330208

2-acetylfluorene NIMAG=0

	x	y	z
h	-0.927800	2.440785	-0.881259
c	1.818016	-1.479804	0.000093
c	2.374231	-0.182617	0.000018
c	1.519015	0.941454	-0.000028
c	0.142231	0.753259	-0.000022
c	-0.405292	-0.553153	-0.000127
c	0.437408	-1.673429	0.000045
h	2.497406	-2.323869	0.000354
h	1.930689	1.945134	-0.000160
h	0.027853	-2.678170	0.000188
c	-0.974015	1.787291	-0.000246
h	-0.927814	2.440645	0.880905
c	-2.225715	0.923070	-0.000048
c	-3.566193	1.304181	0.000013
c	-4.555558	0.308424	0.000073
c	-4.204541	-1.050540	0.000113
c	-2.859832	-1.439826	0.000064
c	-1.871285	-0.448277	-0.000089
h	-3.847914	2.352788	-0.000117
h	-5.602884	0.591795	0.000059
h	-4.983461	-1.805699	0.000222
h	-2.593856	-2.492016	0.000140
c	3.855313	-0.042993	-0.000023
c	4.476847	1.338505	0.000385
h	4.173122	1.910732	-0.883679
h	4.173323	1.910350	0.884789
h	5.561998	1.232714	0.000279
o	4.594445	-1.054807	-0.000382

total energy = -108.2353206