chem-bla-ics

RSC now allows Jmol in main text of publication... well, almost

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Richard Kidd wrote in the ChemistryWorldBlog about Henry Rzepa to have published two papers in RSC journals where Jmol is part of the main paper, after having used Jmol in extra material in ACS journals before. The key here is that the Jmol is part of the official text... when you open the paper in a browser, you immediately get to see the Jmol live, 3D graphics! Well, so it is said in the blog.

However, when I checked the HTML of the first of the two papers (*A computational investigation of the structure of polythiocyanogen*, doi:10.1039/b810147g). The main HTML **still** links to a supplementary page. Progress, but not perfect either:

Table 1 3D coordinates, energies and ELF(π) isosurfaces for polythiocy available in online version

x in $[(SCN)_2]_x$	System	Free energy (relative)[b]	symmetry	Digital Repository[c]
1	-	[-981.9853] 0.0 {-982.0429} 0.0	C_2	Freq NMR Freq
10	3	[-981.9967] -7.2	C_1	Freq NMR
10	5	[-982.0333] -30.1 {-982.0895} -29.2	C_s	Freq NMR Freq
10	6	[-982.0225] -23.3 {-982.0755} -20.5	C_s	Freq NMR Freq
15 ELF[d] ELF[e]	7	[-982.0343] -30.7	C_{1Sh}	Freq NMR
16	8	[-982.0345] -30.9	C_{16h}	NMR
10	9	[-981.9620] +14.6	C_{10}	Freq NMR
5	10	[-982.0410] -35.0	C_1	Freq NMR
6	11	[-982.0438] -36.7	C_2	Freq NMR
6	12	[-982.0275] -26.5	C_2	Freq NMR
7	13	[-982.0432] -36.3	C_1	Freq NMR
8	14	[-982.0407] -34.8	S_4	Freq NMR
9	15	[-982.0438] -36.7	C_s	Freq NMR
10 ELF[f] ELF[g]	16	[-982.0431] -36.3	D_2	Freq NMR
10	17	[-982.0426] -36.0	C_2	Freq NMR

