benzoapyrene A **record** is a folder or a zip file containing: -1) All the NMR spectra of a compound (including 1D spectra Chemical shift (or range in case > <NMREDATA 1D 1H> of overlap or complex multiplet) FID's, acquisition and processing parameters). ; note that integrals (E) were not measured in the spectrum but set **12** location of the spectrum in 2) The .sdf file containing the NMReDATA for Spectrum Location=file:./benzoapyrene/10/pdata/1/\ the folder/zip files Larmor=500.13\ each compound assigned for the sample. 9.0600, L=H(17), S=d, J=8.44(H(19)), E=1.00\ compound1.nmredata..sdf 9.0700, L=H(14), S=d, J=9.13(H(16)), E=1.03 Label (see left) 8.5300, L=H(6), S=s, E=1.03\ 8.3400, L=H(16), S=d, J=9.13(H(14)), E=1.05 "structure" part of the file 8.3000, L=H(18), S=d, J=8.06(H(20)), E=1.02 Wultiplicity ("d" for doublet, etc.) benzo(a)pyrene The format is the same 8.2500, L=H(15), S=d, J=7.65(H(11)), E=1.00 coupling constants. They can be demo of .sdf file containing NMReDATA as .mol files (compatible with 8.1000, L=H(7), S=d, J=7.31(H(11)), E=1.06\ assigned as here: $J_{H(11),H(7)} = 7.31$ Hz test generationV1 1 most chemical structure editor) 20 24 0 0 0 0 0 0 0 0999 V2000 7.9800, L=H(11), S=dd, J=7.31(H(7)), 7.65(H(15)), E=1.02\ -1.65832.2334 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 Integral (crude exp. -0.6633 3.1556 0.0000 C 7.9400, L=H(2), S=d, J=9.07(H(1)), E=1.01values). The rounded -1.37530.8191 0.0000 C 7.8500, L=H(19), S=dd, J=6.77(H(20)), 8.44(H(17)), E=1.05\ number of atom can be 0.7234 2.7603 7.7900, L=H(20), S=dd, J=6.77(H(19)), 8.06(H(18)), E=0.98given following N=) 0.0000 0.3848 0.0000 C For a list of all 1D signal attributes, see: -0.5264-3.37460.0000 C http://nmredata.org/wiki/1D attributes -3.1687-2.4653 0.0000 C > <NMREDATA 1D 13C> -1.5724-4.2723; note that intensisites were not measured in the spectrum 110 for CH -3.81550.0000 C -2.91040 0 0 0 100 for Cq\ 1 2 2 0 0 0 Spectrum Location=file:./benzoapyrene/13/pdata/1/\ 0 0 Larmor=125.0\ For a list of all spectra properties, see: 0 0 Decoupled=1H\ ← list of atoms with coordinates (either http://nmredata.org/wiki/NMReDATA tag format 131.6000, L=(4), I=100.002D as in "flat" structures used for 131.4000, L=(12), I=100.00drawing or 3D) 0 0 131.35, L=(10), I=100.00 Chemical shift in ppm 0 0 list of bonds 129.9, L=(3) I=100.00Label (see the NMREDATA ASSIGNMENT tag) 0 0 0 128.9, L=(18), I=110.00128.17, L=(1), I=110.00\ \leftarrow Signal intensity (usefull to distinguish 128.23, L=(13), I=100.00\ signals in DEPT spectra, to determine the 127.9, L=(2), I=110.00\ sign of the peak and quantidy NOE. Here 127.4, L=(9), I=100.00\ 9 13 127.5, L=(16), I=110.00\ they were set to 100 and 110 but the 126.09, L=(11), I=110.00\ experimental values should be given here.) 126.06, L=(20), I=110.00\ 128.3, L=(8), I=100.00\ 11 15 1 125.97, L=(19), I=110.00\ 12 15 2 0 125.6, L=(15), I=110.0012 16 124.8, L=(6), I=110.00\ 124.9, L=(7), I=110.00\ 13 17 1 Explicit structures (including all hydrogen atoms) 14 16 2 0 0 0 123.8, L=(5), I=100.00should be favored to facilitate the assignment of 17 19 2 0 0 0 123.0, L=(17), I=110.0018 20 2 0 0 0 non-equivalent hydrogens. For aromatic compounds 122.2, L=(14), I=110.0019 20 1 0 0 0 implicit hydrogen is fine. M END 2D spectra Isotope in F1 / type of mixing / isotope in F2 > <NMREDATA_VERSION> "NMReDATA" part of the file > <NMREDATA 2D 1H NJ 1H 1.1 Doi are mandatory for NMR Records Larmor=500.13\ "N": multiple-bond, "J": scalar coupling mixing > <NMREDATA ID> CorType=COSY The zip file of the record can be Doi=10.5281/zenodo.1146869\ Spectrum Location =file:./benzoapyrene/12/1/pdata/1/\ accessed Record=https://zenodo.org/record/1146869/files/sample1.zip\ H(1)/H(2)directly. Path=compound1.nmredata.sdf\ H(7)/H(11) H(11)/H(15)\ The .sdf file can include "tags". > <NMREDATA SOLVENT> H(14)/H(16)\ Each tag has a name between "> <" and ">" Correlation of "H(1)" with "H(2)". cdc13 H(19)/H(20)\ and data (one or more lines terminating with H(19)/H(17)\ an empty line. > <NMREDATA TEMPERATURE> H(20)/H(18)\ NMReDATA tags start with "NMREDATA_". 298.15 13C isotope in F1, 1J mixing, 1H isotope in hdimension This tag associates the labels used > <NMREDATA_ASSIGNMENT> > <NMREDATA 2D 13C 1J 1H> in the assignment and the atom(s) of the (1), 128.1712, 1\ Larmor=500.13\ molecule. (2), 127.9300, 2 CorType=HSQC (3), 129.9, 3Spectrum_Location =file:./benzoapyrene/13/pdata/1/\ (4), 131.6, 4 (1)/H(1)Chemical shifts in ppm (no truncation of the (5), 123.8, 5\ (2)/H(2) chemical shift before the fourth decimal) Link to the spectra (the data must include (6), 124.8, **6**√ (6)/H(6)\ the fid, and the processed data). This points either (7), 124.9, 7(7)/H(7)(8), 128.3, 8(11)/H(11)to a folder where the .sdf file is located or to a Labels used for the assignment (see right column). (9), 127.4, 9(14)/H(14)permanent record in an open-access database. In this example, the proton bound to the atom 1 (10), 131.35, 10(15)/H(15)in the structure part (in blue above) was (11), 126.09, 11(16)/H(16)(12), 131.4, 12called "H(1)" and the carbon labeled "(1)", but the (17)/H(17)Correlation of carbon "(1)" with hydrogen "H(1)". (13), 128.23, 13(18)/H(18)authors can chose the labels according to IUPAC rules (14), 122.2, 14(19)/H(19)or the requirement of the journal where the data are For a list of all 2D signal attributes, see: (15), 125.6, 15(20)/H(20)published. http://nmredata.org/wiki/2D attributes (16), 127.5, 16(17), 123.0, 17 \times For compatibility with SDF libraries, the line $(18), 128.9, 18 \$ HMBC, NOESY data would follow separator of multiple-lines tags is "\" + CR. (19), 125.97, 19\ with the same format (20), 126.06, 20\ > <NMREDATA LITERATURE> Reference to the main publication Reference to the atom number in the .mol block Source=Journal H(1), 8.02, H1associated to the record. H(2), 7.94, H2(see the structure part in the blue frame). DOI=... H(6), 8.53, H6When hydrogen atoms are implicit, the atom number H(7), 8.10, H7to which the hydrogen atom is bound is given Other data such as the origin H(11), 7.98, H11\ > <...> following "H". H(14), 9.07, H14of the sample, the sample Note: H(15), 8.25, H15preparation and other analytics Implicit hydrogen atoms should not be used H(16), 8.34, H16\ data could (and should) be added to .sdf file H(19), 7.85, H19\ when non-equivalent hydrogen of CH2's are outside the NMReDATA initiative. H(20), 7.79, H20unambiguously assigned (as in substituded H(17), 9.06, H17\ cyclohexane derivatives such as menthol). H(18), 8.30, H18\ End of file code \$\$\$\$