Phase shift in polymer SRU

Examples

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|  | Original structure | InChI & InChIKey | Structure as restored from InChI  (after importing xyz-less Molfile to Accelrys Draw 4.1 then making ‘Chemistry->Clean’) | OK? |
| kahovec2002-p1925-ex1.mol |  | InChI=1B/C2H3BrO.2Zz/c3-2-1-4-2;;/h2H,1H2;;/z101-1-4(5,6-1,2,1,4,2,4)  InChIKey=YEUZYGFTWKSHSS-AWQNPEGIBA-N |  | Yes |
| kahovec2002-p1925-ex2.mol |  | InChI=1B/C2H3BrO.2Zz/c3-2-1-4-2;;/h2H,1H2;;/z101-1-4(5,6-1,2,1,4,2,4)  InChIKey=YEUZYGFTWKSHSS-AWQNPEGIBA-N |  | Yes |
| kahovec2002-p1925-ex3.mol |  | InChI=1B/C2H3BrO.2Zz/c3-2-1-4-2;;/h2H,1H2;;/z101-1-4(5,6-1,2,1,4,2,4)  InChIKey=YEUZYGFTWKSHSS-AWQNPEGIBA-N |  | Yes |
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| kahovec2002-p1931-r13-ex1.mol |  | InChI=1B/C10H10O2.2Zz/c11-10-9-5-3-8(4-6-9)2-1-7-12-10;;/h3-6H,1-2,7H2;;/z101-1-12(13,14-1,2,1,7,2,8,7,12,9,10,10,12)  InChIKey=BBWNABGMJALEOQ-ZMZMYGSVBA-N |  | Yes |
| kahovec2002-p1931-r13-ex2.mol |  | InChI=1B/C10H10O2.2Zz/c11-10-9-5-3-8(4-6-9)2-1-7-12-10;;/h3-6H,1-2,7H2;;/z101-1-12(13,14-1,2,1,7,2,8,7,12,9,10,10,12)  InChIKey=BBWNABGMJALEOQ-ZMZMYGSVBA-N |  | Yes |
| kahovec2002-p1931-r13-ex3.mol |  | InChI=1B/C10H10O2.2Zz/c11-10-9-5-3-8(4-6-9)2-1-7-12-10;;/h3-6H,1-2,7H2;;/z101-1-12(13,14-1,2,1,7,2,8,7,12,9,10,10,12)  InChIKey=BBWNABGMJALEOQ-ZMZMYGSVBA-N |  | Yes |
| gishurst15\_1.mol |  | InChI=1B/C3H5NO.2Zz/c5-3-1-2-4-3;;/h1-2H2,(H,4,5);;/z101-1-5(6,7-1,2,1,3,2,4,3,4)  InChIKey=WJNTXTLLURMHBY-DJONAFDXBA-N |  | Yes |
| gishurst15\_2.mol |  | InChI=1B/C3H5NO.2Zz/c5-3-1-2-4-3;;/h1-2H2,(H,4,5);;/z101-1-5(6,7-1,2,1,3,2,4,3,4)  InChIKey=WJNTXTLLURMHBY-DJONAFDXBA-N |  | Yes |
| gishurst15\_3.mol |  | InChI=1B/C3H5NO.2Zz/c5-3-1-2-4-3;;/h1-2H2,(H,4,5);;/z101-1-5(6,7-1,2,1,3,2,4,3,4)  InChIKey=WJNTXTLLURMHBY-DJONAFDXBA-N |  | Yes |
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|  | gishurst15\_1.mol FixedH |  |  |  |
|  | gishurst15\_2.mol FixedH |  |  |  |
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| CHEBI 27602 |  | InChI=1B/C12H26O16P2/c13-1-6(15)3-25-30(22,23)26-5-7(4-24-29(19,20)21)27-12-11(18)10(17)9(16)8(2-14)28-12/h6-18H,1-5H2,(H,22,23)(H2,19,20,21)/z101-2,4-5,7-12,14,16-19,21,24,26-29(20-29,30-26)/t6?,7?,8-,9-,10+,11-,12+/m1/s1  InChIKey=CVGGAOGCVJSXBB-OHILBRHSBA-N |  |  |
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