Supplementary Material

The synthesis of new functionalized 1,3,5-triazine-based stable bi- and trinitroxides of the 2,5-dihydroimidazole series

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**Spectrum 20.** $^{13}$C NMR (DMSO-$d_6$) spectrum of compound 7
Spectra 17-20 represent $^1$H (400 MHz) and $^{13}$C (100 MHz) spectra recorded for the DMSO-$d_6$ solutions of 7 and 8. The only difference in the chemical structures of these two compounds is that the H-4‴ atom in 8 is replaced to benzyl substituent in 7. Both compounds have been obtained through the condensation of the corresponding hydroxylaminoketone and 4-(4-hydroxyphenyl)cyclohexanone (6) in presence of ammonium acetate in methanol saturated with ammonia. As compound 8 has been already determined to be trans-ee-isomer on the base of analysis of its $^1$H, $^{13}$C, NOESY and ROESY NMR spectra supporting with the quantum chemical conformational analysis data\textsuperscript{1}, and the $^1$H and $^{13}$C NMR spectra of the similar fragments of these two compounds have the similar chemical shifts and coupling constants, it is reasonable to suggest that the geometry of 7 was similar to 8. Finally, compound 8 has been also determined to be trans-ee-isomer.
Spectrum 21. $^1$H NMR (CDCl$_3$+DMSO-$d_6$) spectrum of compound cis-14

Spectrum 23. $^1$H NMR (CDCl$_3$+DMSO-$d_6$) spectrum of compound cis-13
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Spectra 21-28 represent $^1$H (400 MHz) and $^{13}$C (100 MHz) spectra recorded for the CDCl$_3$+DMSO-$d_6$ solutions of cis-13, trans-13 and cis-14 and trans-14. Only the side parts of the molecules are different, but the main skeletons are the same. All the compounds have been synthesized through the similar synthetic way: condensation of the corresponding hydroxylaminoketone and 4-hydroxycyclohexanone in presence of ammonium acetate in methanol saturated with ammonia, following oxidation by means manganese dioxide and Mitsunobu acylation of the obtained derivatives using 4-alkoxysubstituted benzoic acid or 3,4,5-alkoxysubstituted benzoic acid, correspondingly. As cis-14 and trans-14 have been already determined to be cis-ea- and trans-ee-isomers on the base of analysis of their $^1$H, $^{13}$C, NOESY and ROESY NMR, and the $^1$H and $^{13}$C NMR spectra of the similar fragments of these two compounds have the similar chemical shifts and coupling constants, it is reasonable to suggest that the geometry of cis-13 was similar to cis-14 and the geometry of trans-13 was similar to trans-14, correspondingly. Finally, compounds cis-13 and trans-14 have been determined to be cis-ea- and trans-ee-isomers, correspondingly.
### Phase transition data

<table>
<thead>
<tr>
<th>Compound</th>
<th>Phase transition data</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>trans</em>-4</td>
<td>Cr₁78 (2) Cr₂ 96 (15) I</td>
</tr>
<tr>
<td><em>trans</em>-5</td>
<td>Cr 82 (20) I</td>
</tr>
<tr>
<td><em>cis</em>-5</td>
<td>Cr 62 (23) I</td>
</tr>
<tr>
<td>1b</td>
<td>-</td>
</tr>
<tr>
<td>1c</td>
<td>Cr 3 (10) I</td>
</tr>
<tr>
<td>2b</td>
<td>Cr 50 (9) I</td>
</tr>
<tr>
<td>2c</td>
<td>Cr 72 (14) I</td>
</tr>
<tr>
<td>15b</td>
<td>-</td>
</tr>
<tr>
<td>15c</td>
<td>Cr 17 (13) I</td>
</tr>
</tbody>
</table>

**Table S1.** Transition temperatures (°C) and enthalpies (kJ/mol, in italics) determined by DSC (5 °C /min) in the heating mode: Cr = crystal; I = isotropic in the temperature intervals from 25 °C to 140 °C for *trans*-4, *trans*-5, *cis*-5, 1b, 15b, and 2c and from -10 °C to 80 °C for 1c, 15c and 2b.
   http://dx.doi.org/10.3998/ark.5550190.p008.808
   http://dx.doi.org/10.1007/s10593-014-1571-7