Supporting Information

Di(1H-tetrazol-5-yl)methanone oxime and 5,5'-(hydrazonomethylene)bis(1H-tetrazole) and their salts: a family of highly useful new tetrazoles and energetic materials

Deepak Chand, a Damon A. Parrish, b and Jean’ne M. Shreeve a

a Department of Chemistry, University of Idaho, Moscow, ID 83844-2343, USA
b Naval Research Laboratory, Code 6030, Washington, D.C. 20375-5001, USA

E-mail: jshreeve@uidaho.edu; Fax: +1-208 885-9146

Table of Contents

Computational data and isodesmic reactions

Ab initio computational data for nine new compounds

1H NMR and 13C NMR spectra of compounds 1–13.

DSC scans of compounds 1–13.

Computational data

All ab initio calculations were carried out by using the Gaussian 03 (Revision D.01) suite of programs. The geometric optimization of the structures and frequency analyses were accomplished by using the B3LYP with the 6-31+G** basis set, and single-point energies were calculated at the MP2/6-311++G** level. Atomization energies were calculated by the G2 method. All of the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies. The remaining task is to determine the heats of formation of these new energetic compounds, which are computed by using the method of isodesmic reactions (Scheme S1).
Scheme S1. Isodesmic reactions
Table 1 Ab initio computational values

<table>
<thead>
<tr>
<th></th>
<th>$E_0^a$</th>
<th>$ZPE^b$</th>
<th>$H_T^c$</th>
<th>$HOF^d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$N $\text{HN=NH}$ H$_2$N</td>
<td>-682.28432</td>
<td>0.0965424</td>
<td>0.010916</td>
<td>674.5243486</td>
</tr>
<tr>
<td>H$_2$N $\text{HN=NH}$ $\text{NH}_2$</td>
<td>-662.45924</td>
<td>0.10931232</td>
<td>0.010815</td>
<td>730.5033453</td>
</tr>
<tr>
<td>H$_2$N $\text{HN=NH}$ $\text{OH}$</td>
<td>-681.18548</td>
<td>0.07139328</td>
<td>0.010259</td>
<td>545.2200254</td>
</tr>
<tr>
<td>H$_2$N $\text{HN=NH}$ $\text{NH}_2$</td>
<td>-661.32701</td>
<td>0.08389344</td>
<td>0.01054</td>
<td>720.4415699</td>
</tr>
<tr>
<td>H$_2$N $\text{HN=NH}$ $\text{NH}_2$</td>
<td>-445.65669</td>
<td>0.123912</td>
<td>0.009482</td>
<td>650.9953919</td>
</tr>
<tr>
<td>H$_2$N $\text{HN=NH}$ $\text{NH}_2$</td>
<td>-429.60242</td>
<td>0.13405</td>
<td>0.010309</td>
<td>654.2531447</td>
</tr>
</tbody>
</table>

$^a$Total energy calculated by B3LYP/6-31+G**//MP2/6-31++G** method (Hartree/Particle); $^b$ zero-point correction (Hartree/Particle); $^c$ thermal correction to enthalpy (Hartree/Particle); $^d$ heat of formation (kJ/mol).
NMR Spectra

Fig: $^{13}$C NMR of 1
Fig: IR of 1

Fig: DSC of 1
Fig: $^1$H NMR of 2
Fig: $^{13}$C NMR of 2
Fig: DSC of 2

Fig: IR of 2
Fig: $^{13}$C NMR of 3
Fig: $^1$H NMR of 3

Fig: IR of 3
Sample: ammoniumsaltsbisnitrosolet
Size: 0.1000 mg
Method: Ramp
Comment: ammoniumsaltsbisnitrosolet

Fig: DSC of 3
Fig: $^{13}$C NMR of 4
Fig: $^1$H NMR of 4
Fig: DSC of 4
Fig: $^{13}$C NMR of 5
Fig: $^1$H NMR of 5
Fig : DSC of 5
Fig: IR of 5

Fig: $^{13}$C NMR of 6
Fig: $^1$H NMR of 6
Sample: aminoguanidiniumsalts crystals
Size: 1.1000 mg
Method: Ramp

File: C:\aminoguanidiniumsalts crystals\01
Operator: deepak
Run Date: 09-Mar-2013 12:35
Instrument: DSC Q10 V9.9 Build 303

Fig: DSC of 6

Fig: IR of 6
Fig. 1: $^1$H NMR of 7
Fig : $^{13}$C NMR of 7
Fig: DSC of 7

Fig: IR of 7
Fig: $^1$H NMR of 8
Fig: $^{13}$C NMR of 8
Fig: DSC of 8

Fig: IR of 8
Fig: $^1$H NMR of 9
Fig: $^{13}$C NMR of 9
Fig: DSC of 9
Fig: IR of 9

Fig: $^1$H NMR of 10
Fig: $^{13}$C NMR of 10

Fig: IR of 10
Fig: DSC of 10
Fig: $^1$H NMR of 11
Fig: $^{13}$C NMR of 11

Fig: DSC of 11
Fig: IR of 11

Fig: $^{13}$C NMR of 12
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A
This journal is © The Royal Society of Chemistry 2013

Fig : $^1$H NMR of 12

Fig : IR of 12
Fig: DSC of 12
Fig: $^1$H NMR of 13
Fig: $^{13}$C NMR of 13

Fig: IR of 13
Fig: DSC of 13