

## Supporting Information

### 1,3-Diazido-2-(azidomethyl)-2-propylammonium salts

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### $^{15}\text{N}$ NMR Spectra

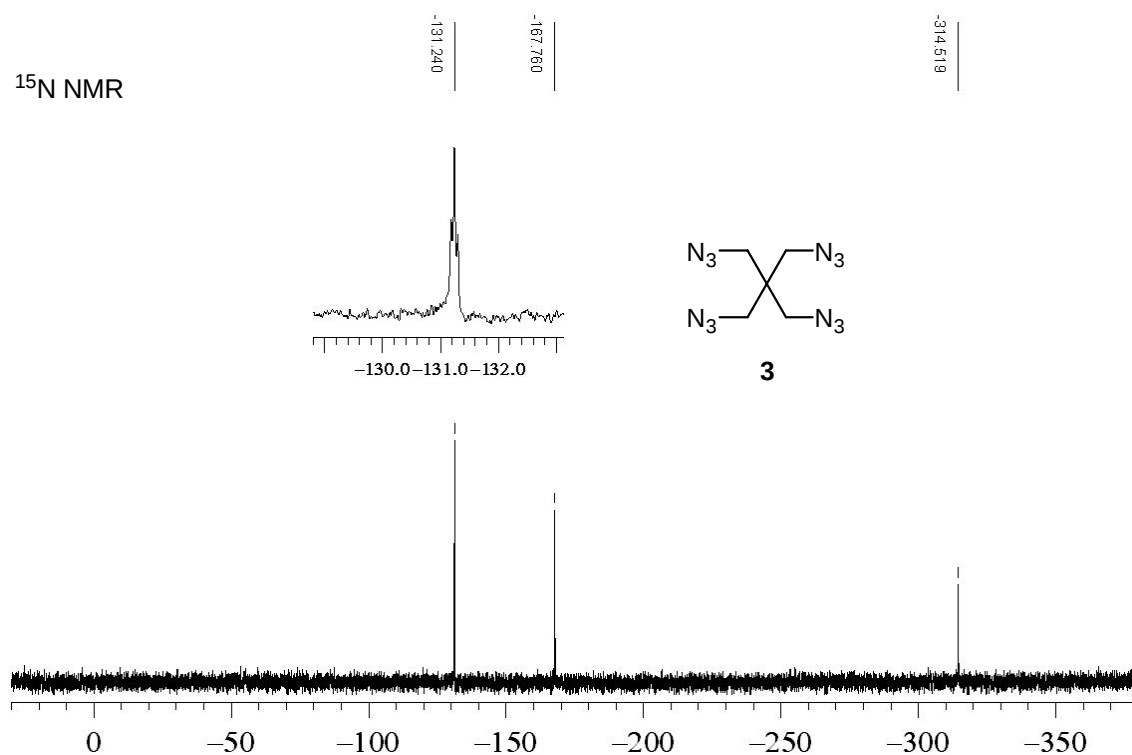


Figure S1

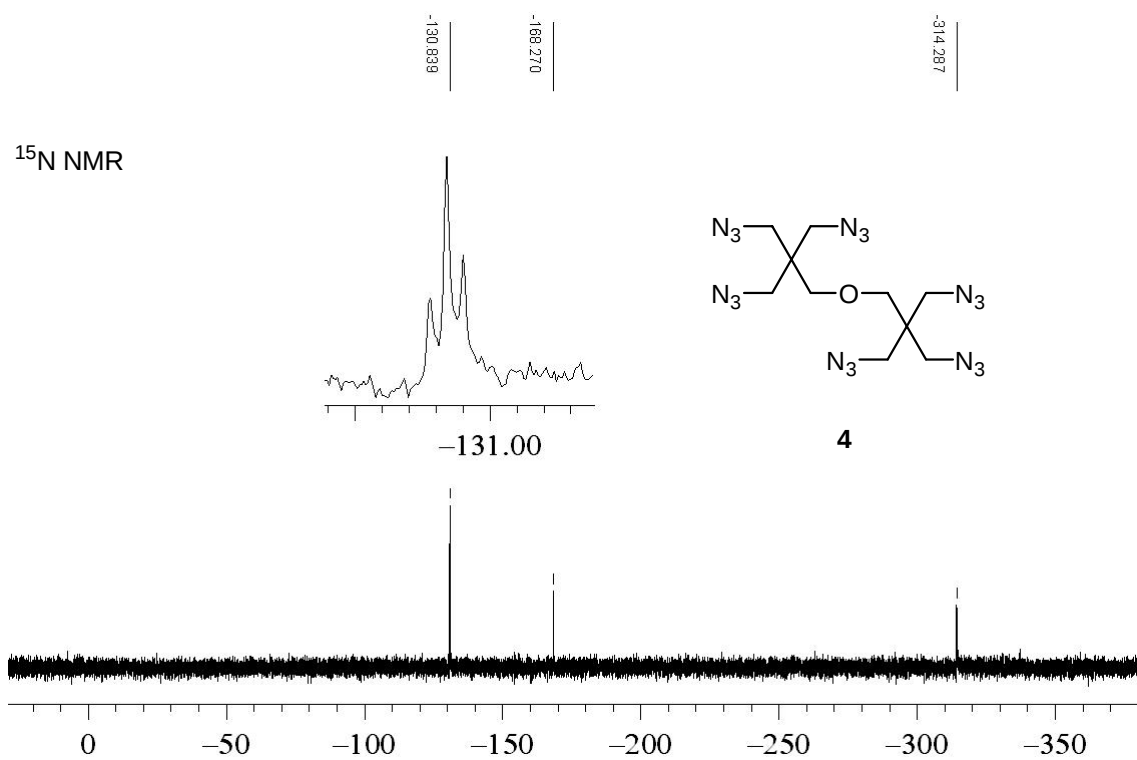


Figure S2

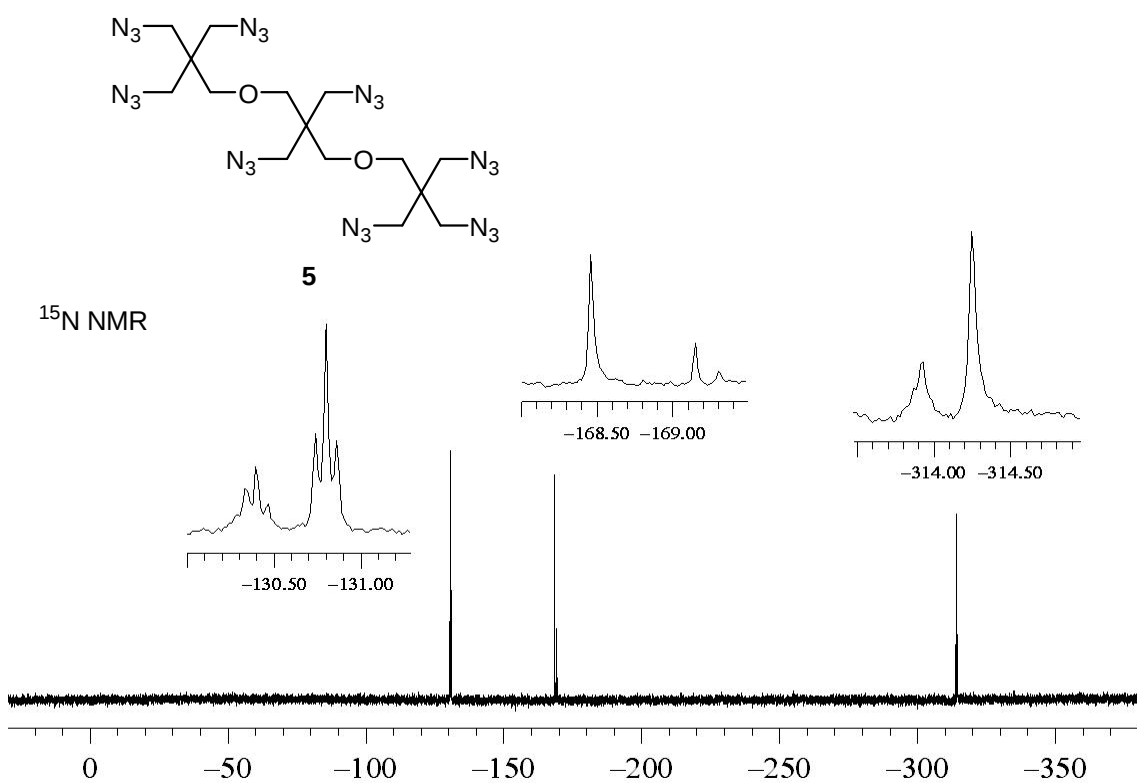


Figure S3

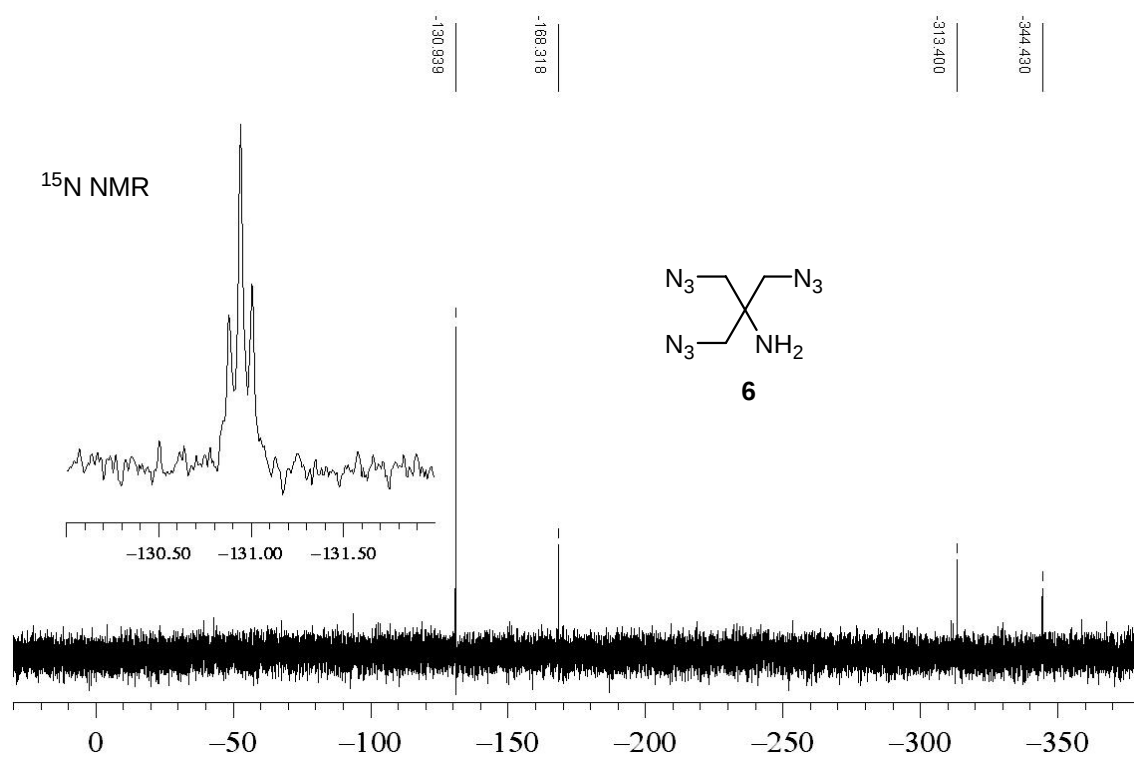


Figure S4

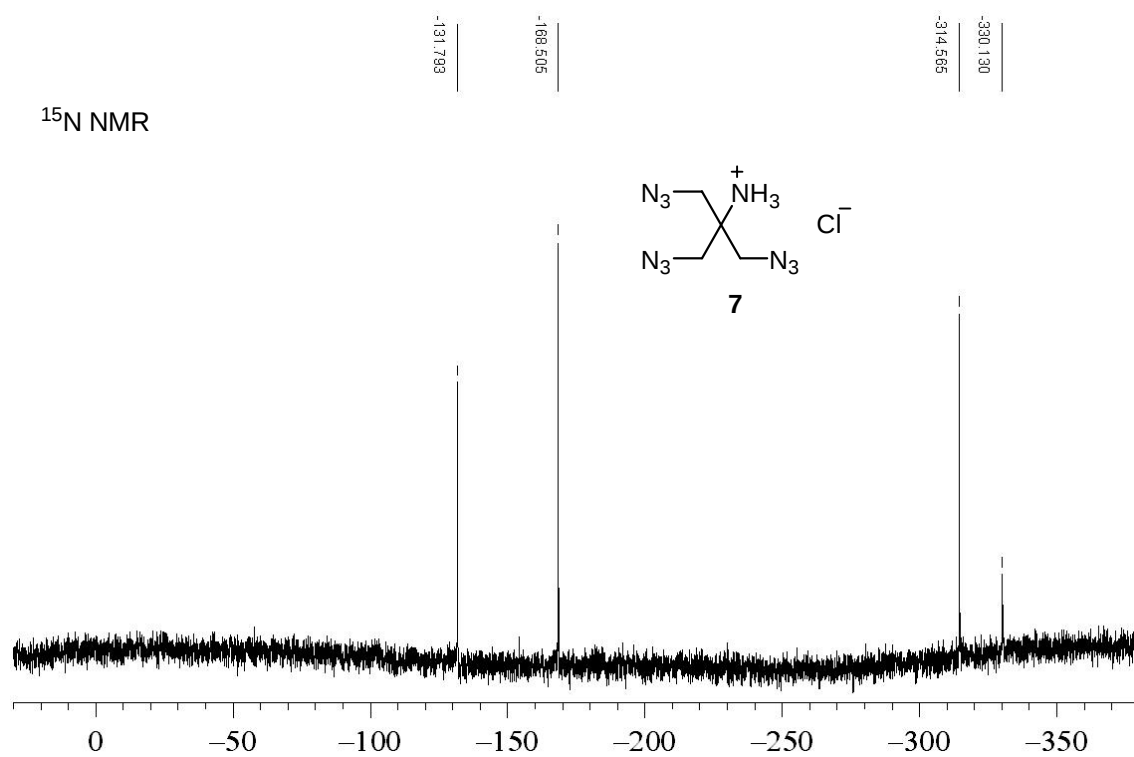


Figure S5

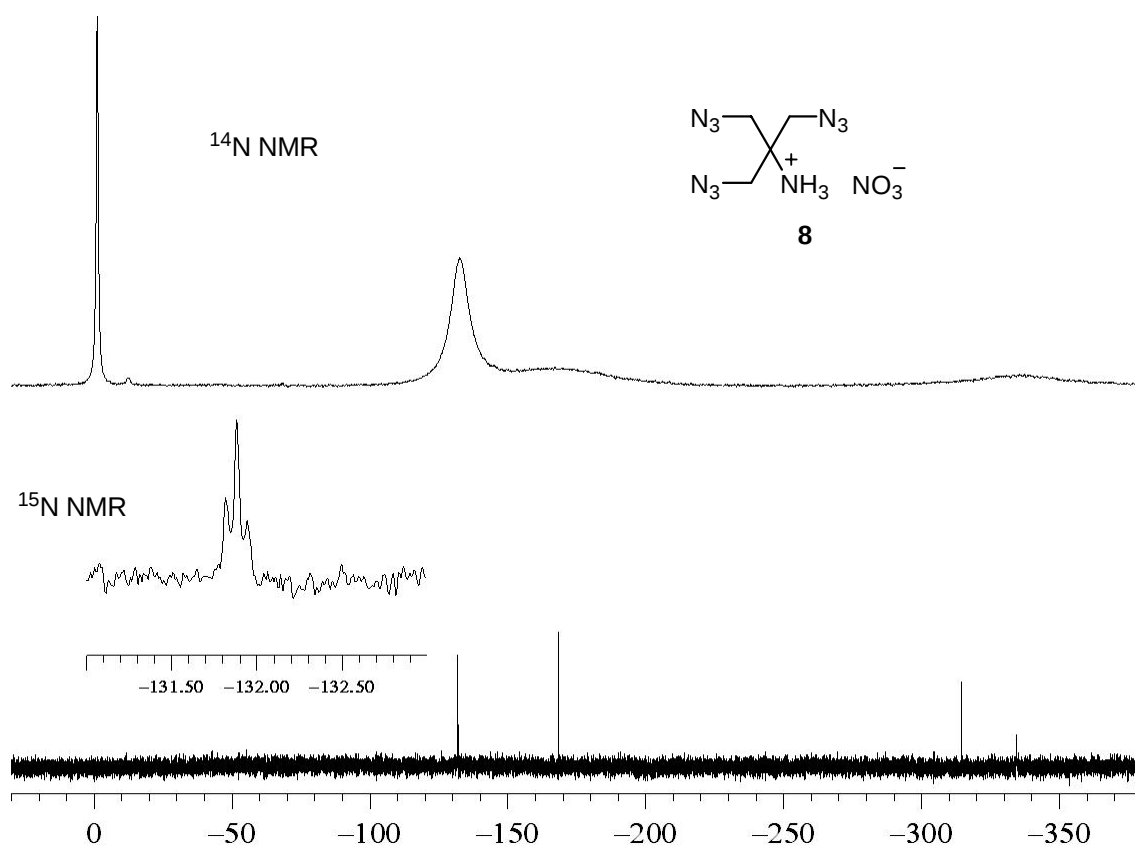


Figure S6

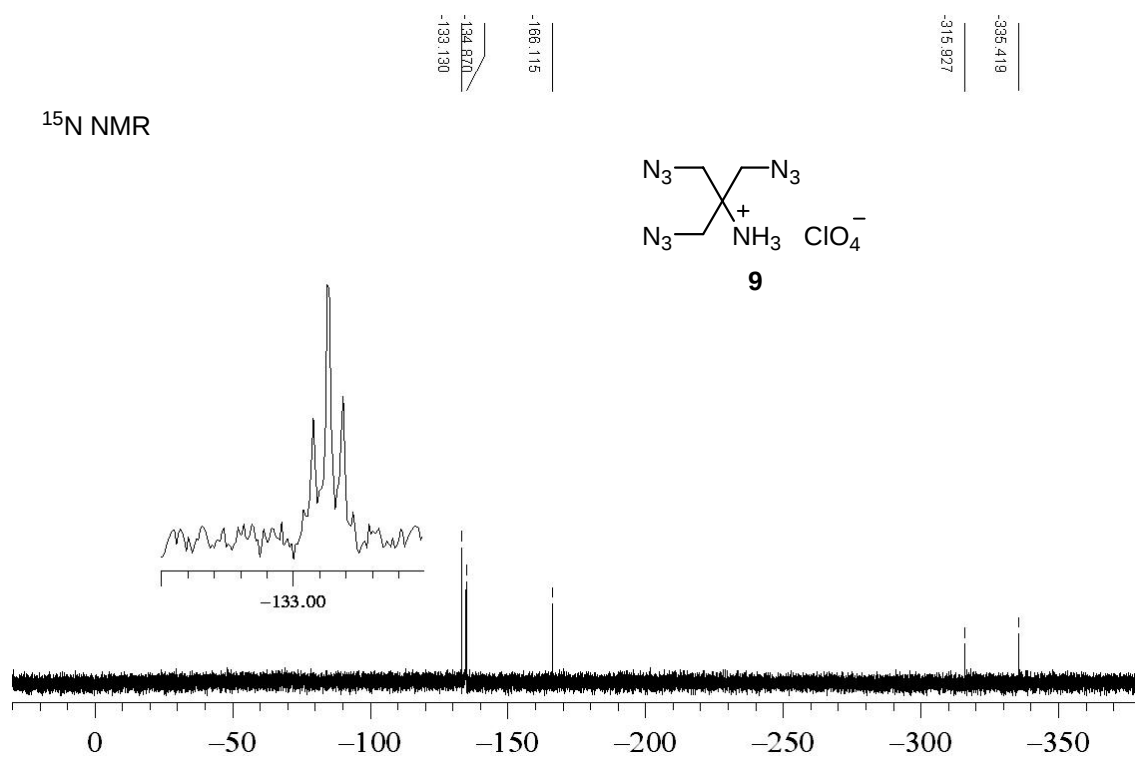


Figure S7

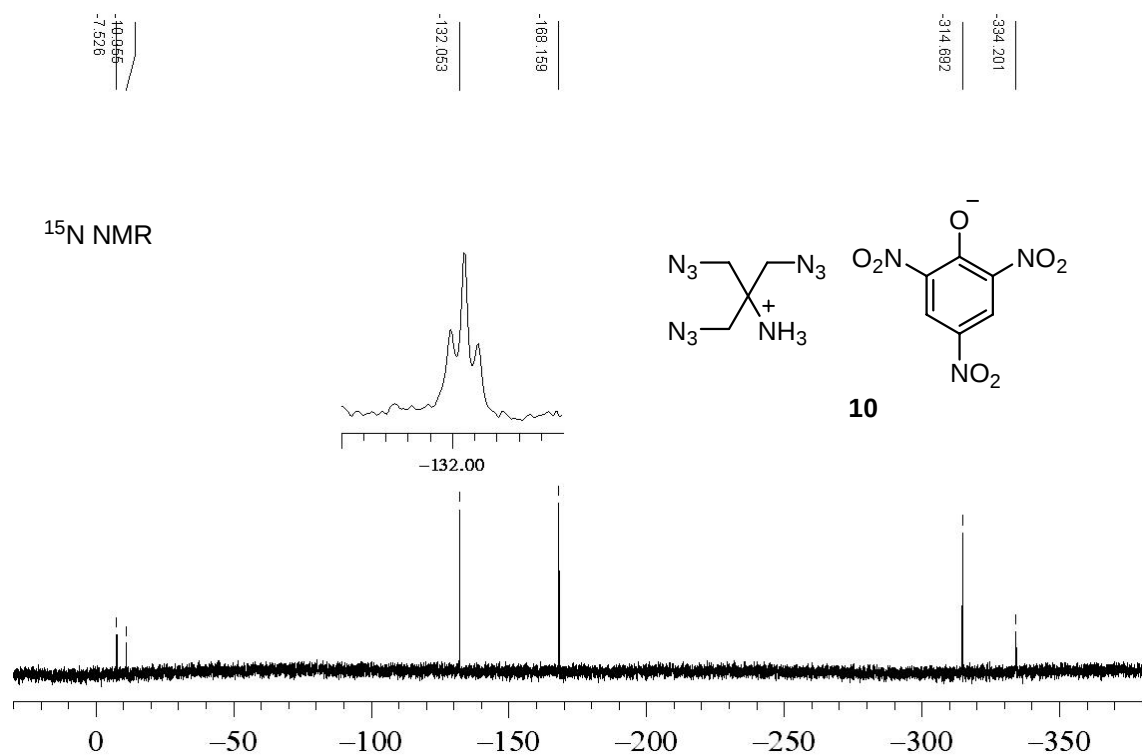


Figure S8

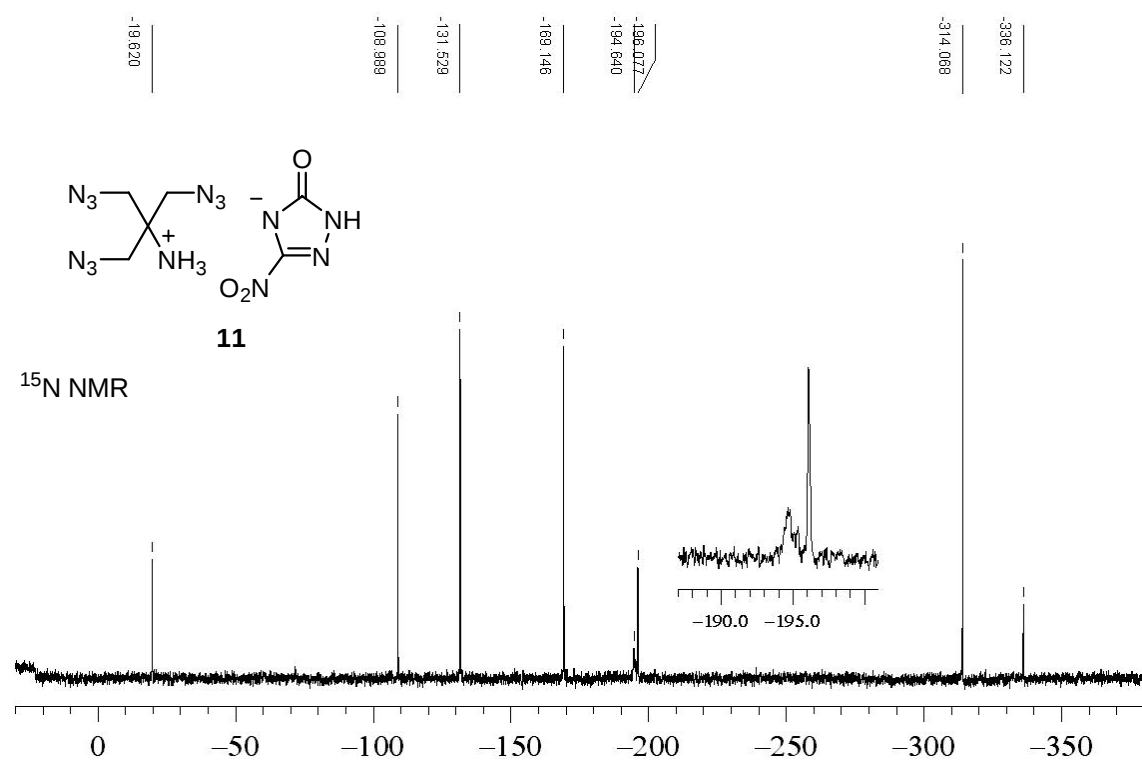


Figure S9



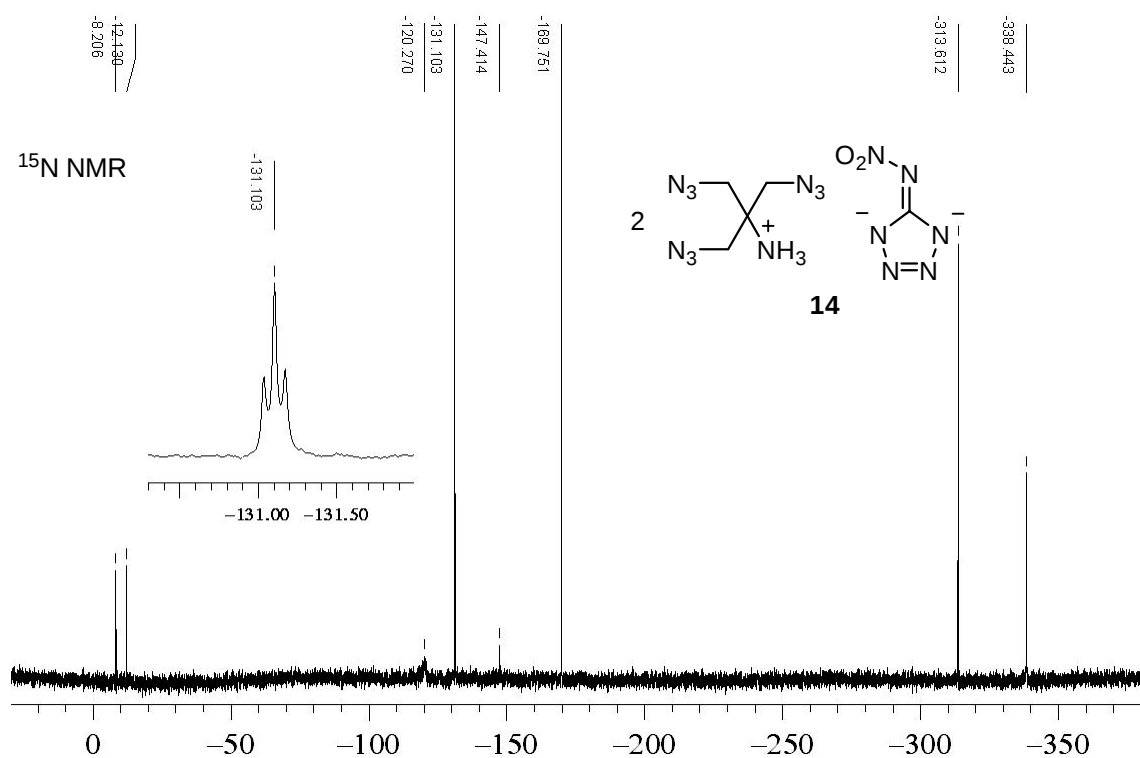


Figure S12

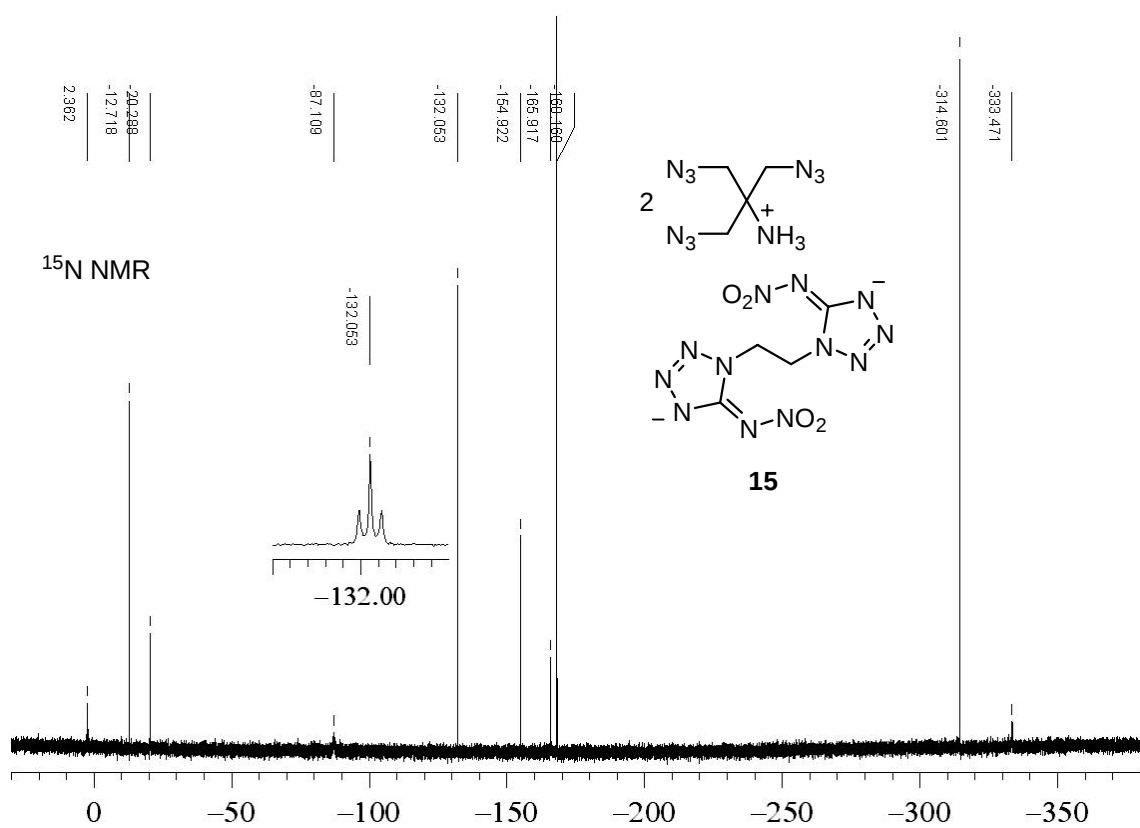


Figure S13

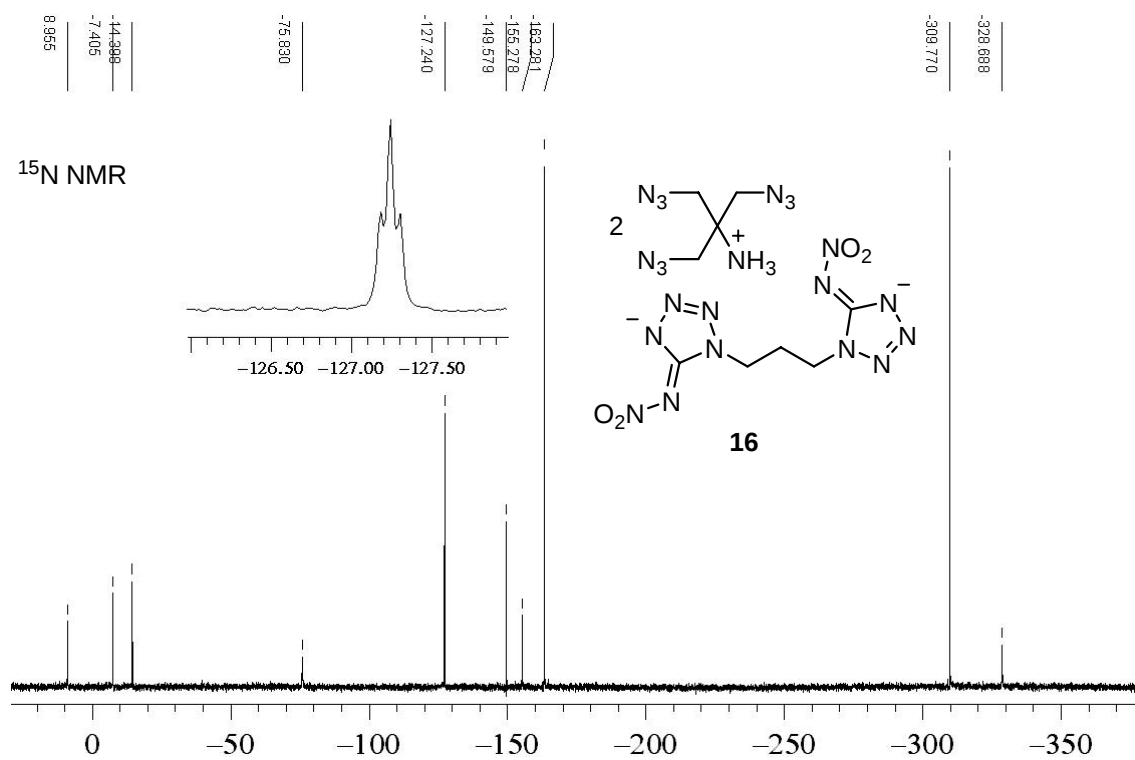


Figure S14

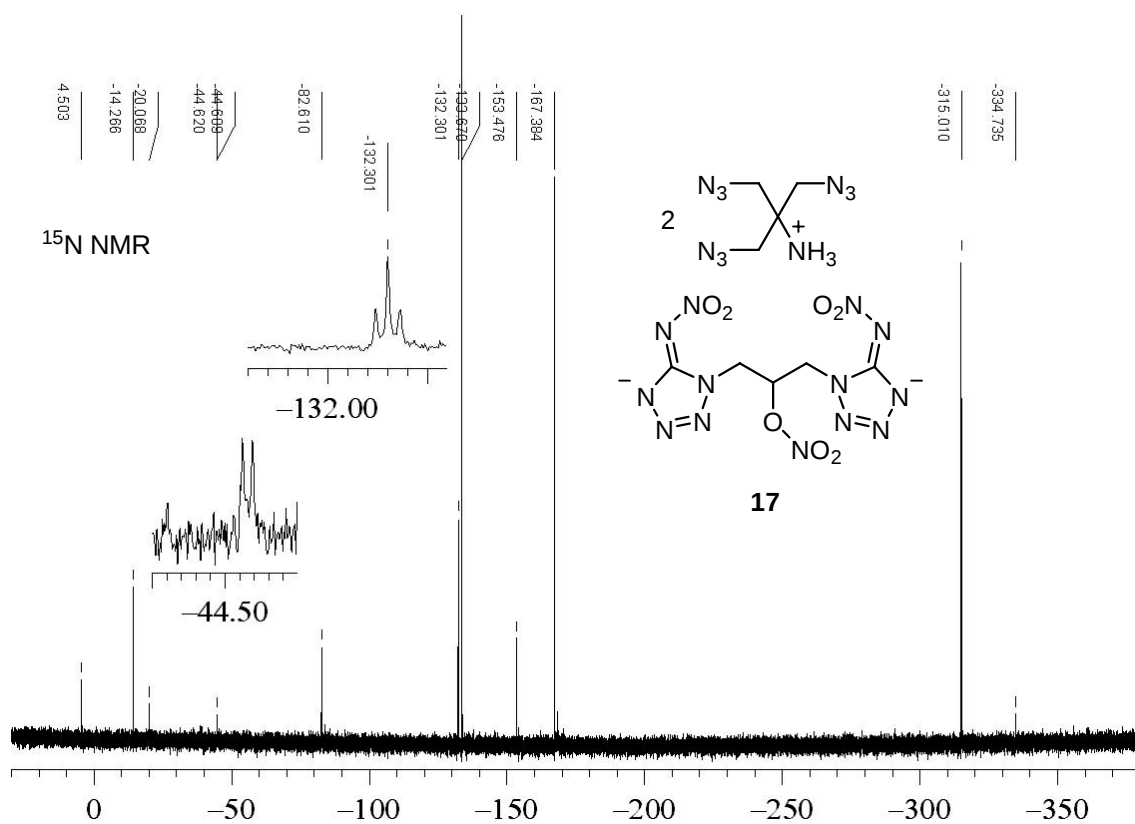


Figure S15

<sup>15</sup>N NMR

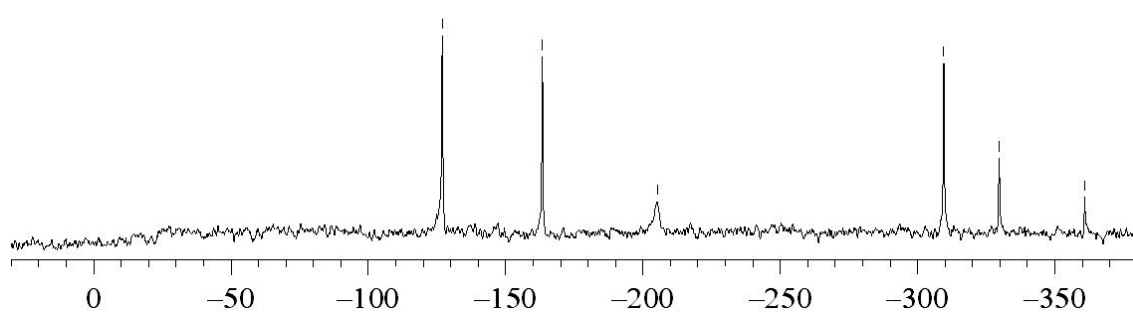
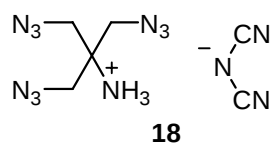


Figure S16

<sup>15</sup>N NMR

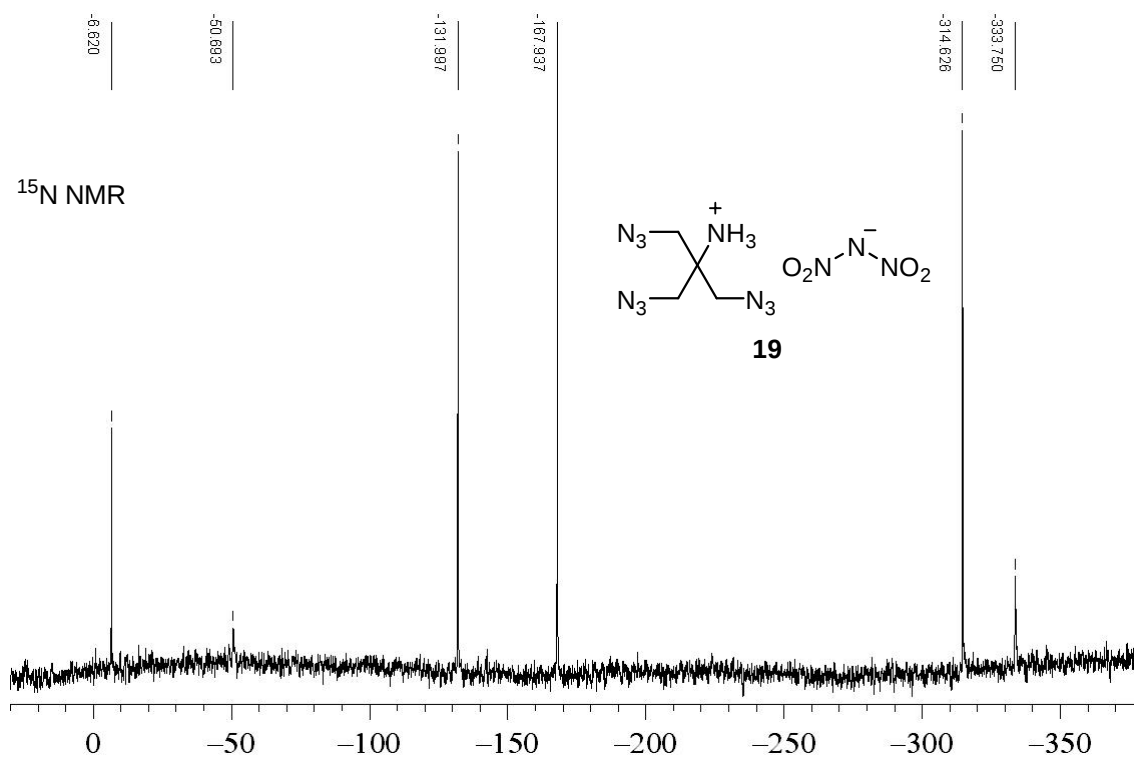
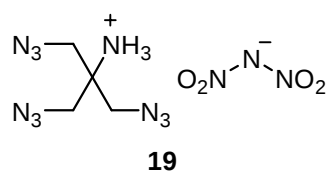
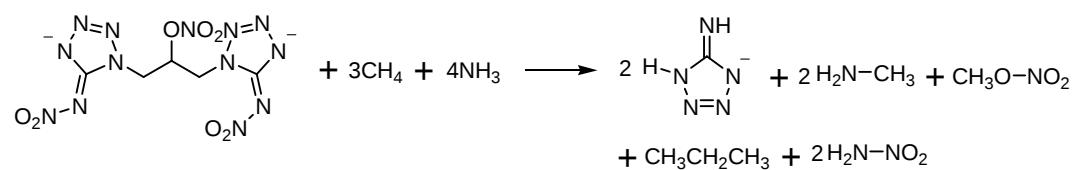
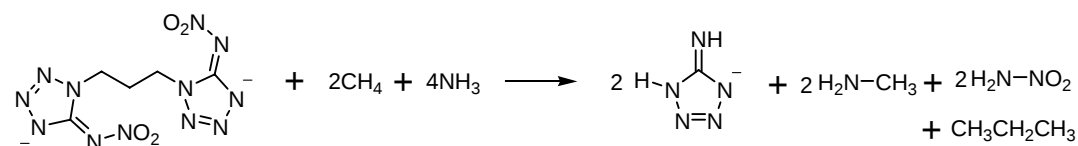
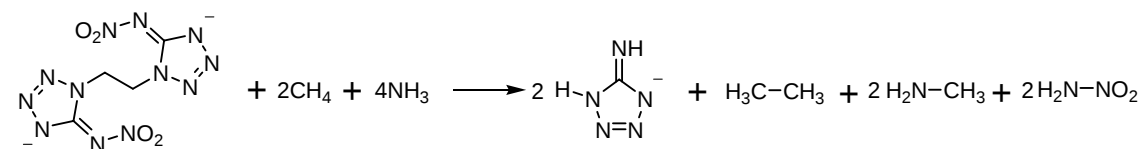
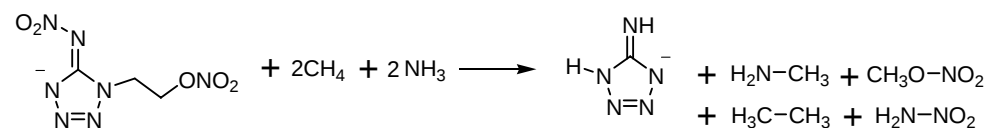
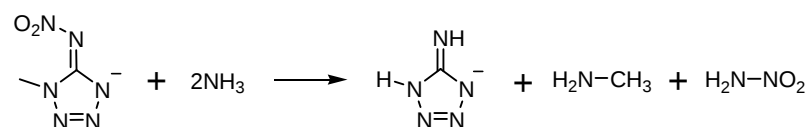
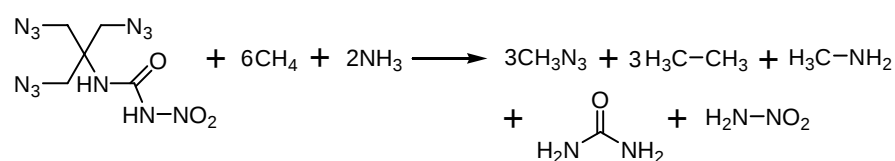
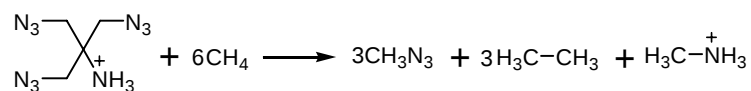
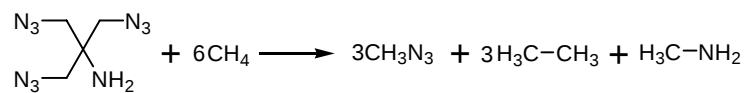


Figure S17

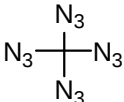
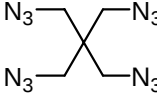
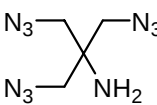
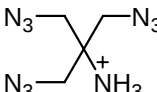
## Computational data

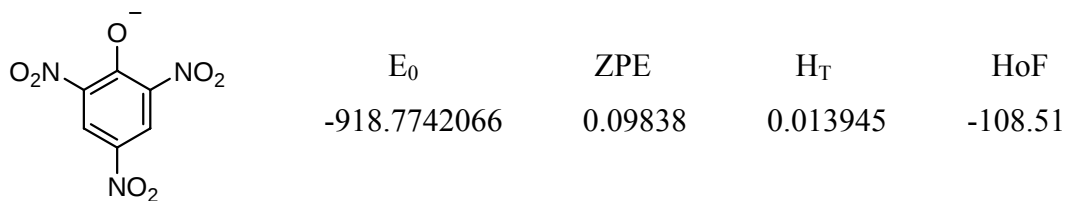
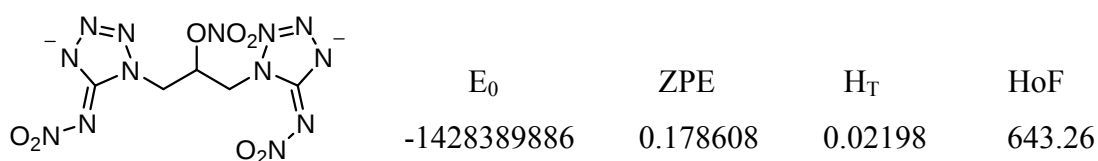
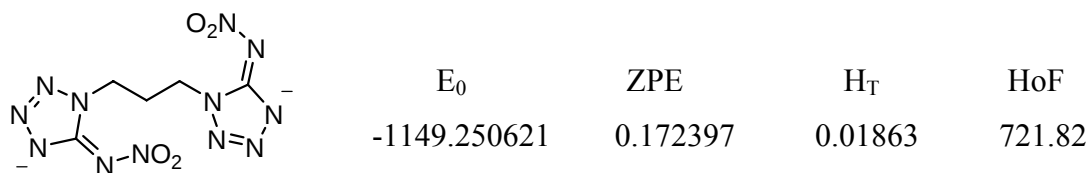
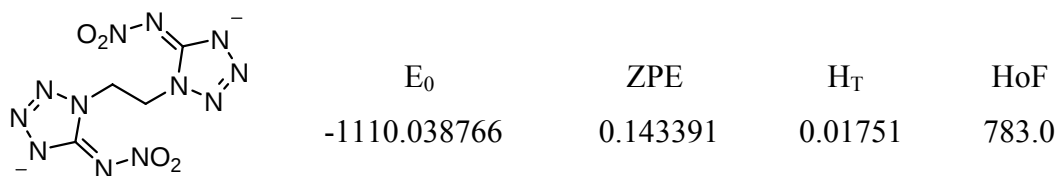
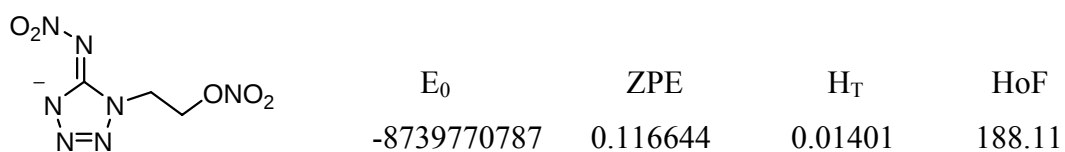
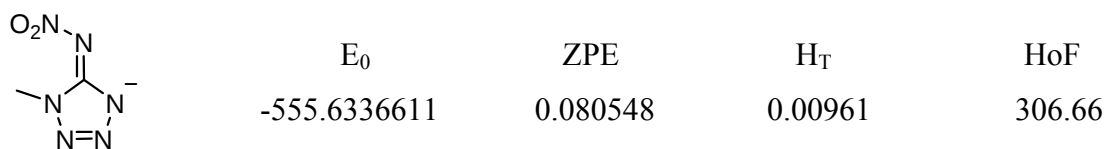
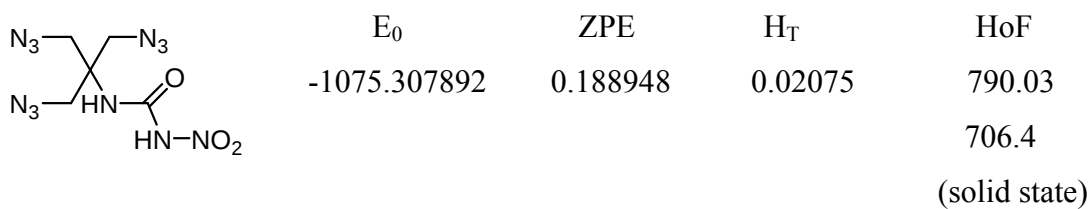


Scheme S1.

The remaining task is to determine the heats of formation of the azide compounds **1**, **3** and **6–20**; these values of 1,3-diazido-2-(azidomethyl)-2-propylammonium cation and nitroiminotetrazole anion were computed by using the method of isodesmic reactions (**Scheme S1**). Calculations were carried out by using the Gaussian 03 (Revision D.01) suite of programs.<sup>1</sup> The geometric optimization of the structures and frequency analyses were carried out by using the B3LYP functional with the 6-31+G\*\* basis set, and single-point energies were calculated at the MP2/6-311++G\*\* level.

Calculated (B3LYP/6-31+G\*\*//MP2/6-311++G\*\*) Total Energy ( $E_0$ ), Zero Point Energy (ZPE), Values of Thermal correction ( $H_T$ ), and Heats of Formation (HoF) [kJ/mol] of the compounds.

|                                                                                     |              |          |         |               |
|-------------------------------------------------------------------------------------|--------------|----------|---------|---------------|
|   | $E_0$        | ZPE      | $H_T$   | HoF           |
|                                                                                     | -693.3339341 | 0.059156 | 0.01260 | 1286.89       |
|                                                                                     |              |          |         | 1203.2        |
|                                                                                     |              |          |         | (solid state) |
|  | $E_0$        | ZPE      | $H_T$   | HoF           |
|                                                                                     | -850.1140375 | 0.174408 | 0.01819 | 1215.67       |
|                                                                                     |              |          |         | 1132.0        |
|                                                                                     |              |          |         | (solid state) |
|  | $E_0$        | ZPE      | $H_T$   | HoF           |
|                                                                                     | -702.9040734 | 0.160121 | 0.01533 | 917.59        |
|                                                                                     |              |          |         | 833.9         |
|                                                                                     |              |          |         | (solid state) |
|  | $E_0$        | ZPE      | $H_T$   | HoF           |
|                                                                                     | -260.5457263 | 0.160121 | 0.01533 | 566.7         |



## Reference

- (1) Gaussian 03, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, Gomperts, J.; R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, **2004**.