Supplementary information

Gurney and cylinder wall velocities of explosives: analytical estimates and thermochemical simulations

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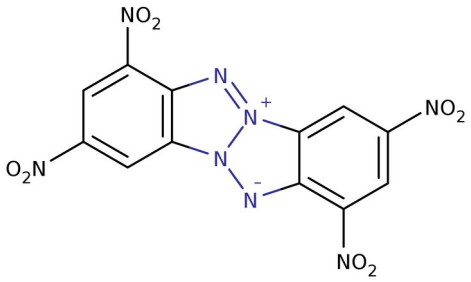
Section S1. Deviations between experiment and calculations for TACOT

An mentioned in section 3.2 of the article, among organic high explosives, TACOT stands out for its specially large deviations between the reported experimental Gurney velocity of 2.12 km/s on one hand, and the calculated values (2.29 km/s using Cγ and 2.34 km/s using EXPLO5) on the other hand. A reviewer suggested that the reported experimental value of 2.12 km/s, which was taken from the LLNL Explosives Handbook of B. M. Dobratz and P. C. Crawford (ref.7), is likely the prompt value of the Gurney velocity, and not the terminal value.



structure of TACOT

This suggestion relies on cylinder wall velocity (v_s) measurements for RX-27-AD, an explosive made essentially of TACOT (92.5%) with 7.5 Kel-F as binder. The values of v_s obtained for expansion ratios of 2.2 and 6.5 are respectively 1.187 and 1.377 km/s, as summarized in Table S1. Using the loading density ρ_0=1.638 g/cc and applying Eq.(5) of the article, this data can be converted to prompt and terminal values of the Gurney velocity of respectively 2.04 and 2.37 km/s. Therefore, the terminal Gurney velocity of pure TACOT should be close to 2.37 km/s, and probably greater as it does not contain any binder that would decrease its performance. Such a value would be also close to the calculated values of 2.29 and 2.34 km/s.

Table S1.Gurney velocities and cylinder wall velocities for RX-27-AD and pure TACOT.

	RX-27-AD experimental velocities		Gurney velocities of pure TACOT		
Expansion ratio V/V_0	Cylinder wall velocity v_s (km/s)	Gurney velocity u_G (km/s)	ref.7 (km/s)	Cγ value (km/s)	EXPLO5 value (km/s)
2.2	1.187	2.04	2.12 ?		
6.5	1.377	2.37		2.29	2.34

Therefore, the experimental value of 2.12 km/s reported for pure TACOT is probably not the terminal value, being lower than the corresponding value obtained for RX-27-AD from cylinder test experiments. On the other hand, it is slightly larger than the prompt value reported for this formulation, which strongly suggests than this value is actually a prompt value rather than a terminal value.

Section S2. Further validation of Cy against third-party data

In addition to Gurney velocity data considered in developing and validating the EXPLO5 procedure (refs 11-12 of the main article), a reviewer pointed to miscellaneous sources from which additional u_G data may be retrieved, along with corresponding formation enthalpy ($\Delta_f H^0$) and density (ρ) data. This valuable data is compiled in Table S2. The structures and $\Delta_f H^0$ of the constitutive species may be found in Table S3, along with references for $\Delta_f H^0$ values not provided in the sources mentioned in Table S2.

Table S2.Gurney velocities and formation enthalpies of additional explosives not considered in earlier studies.[10-13] Units: $\Delta_f H^0$ in (kJ/mol), ρ in g/cc and u_G values in km/s. The numbers in square brackets correspond to article reference numbers where this data are to be found, along with the definition of the materials. This data was indicated by the reviewer and taken from ref.7 of the paper whenever available, or calculated from the chemical composition of the material and the formation enthalpies is its component molecules.

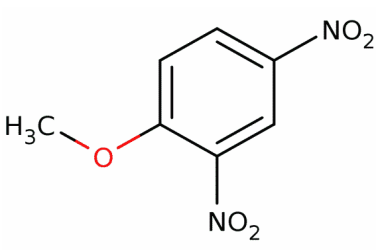
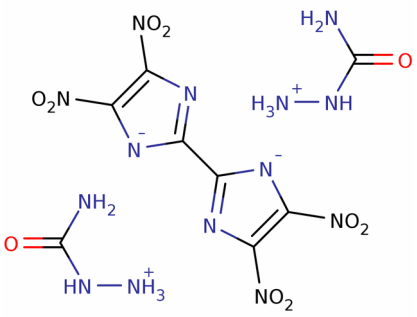
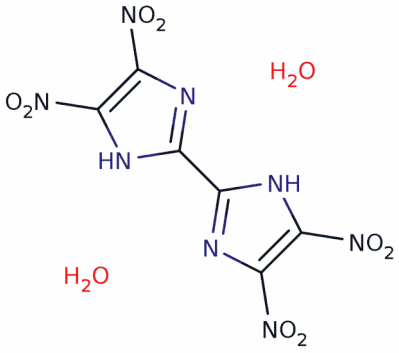
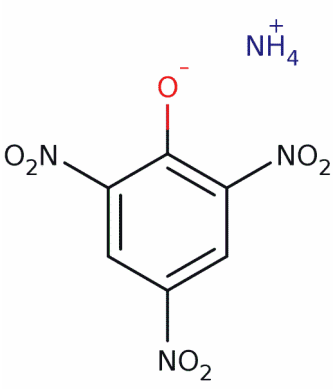
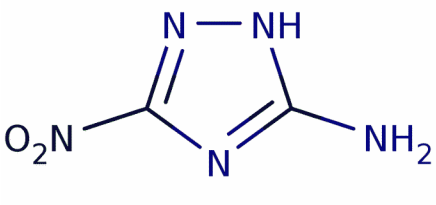
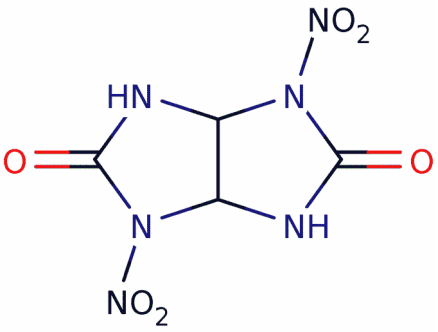
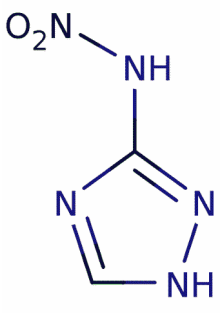
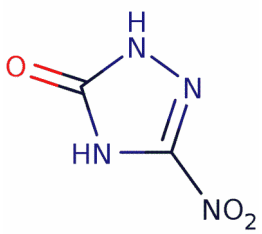
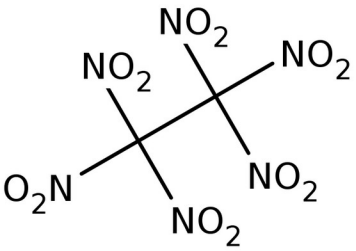
Explosive	Stoichiometry	$\Delta_f H^0$	ρ	u_G expe.	u_G calc.
DNAN	$C_7H_6N_2O_5$	-186.65	1.45	2.00 [39]	1.969
SK TNBI	$C_8H_{12}N_{14}O_{10}$	-414	1.55	2.14 [40]	2.187
TNBI.2H_2O	$C_6H_6N_8O_{10}$	-115	1.72	2.62 [40]	2.661
NTO	$C_2H_2N_4O_3$	-100.71	1.77	2.37 [41]	2.310
RX-45-AA [a]	$C_{1.570}H_{2.233}N_{3.682}O_{1.473}Cl_{0.036}$	15.77	1.752	2.31 [42]	2.216
AmPicCC [b]	$C_{3.043}H_{3.554}N_{1.402}O_{2.519}$	-147.7	1.481	2.13 [43]	2.091
DINGU/HNE/wax (63/32/5)	$C_{1.657}H_{1.800}N_{2.269}O_{2.909}$	-47	1.63	2.32 [44]	2.612
NTO/HNE/wax (76/19/5)	$C_{1.652}H_{1.882}N_{2.717}O_{2.513}$	-52	1.752	2.49 [44]	2.503
NITRA	$C_2H_3N_5O_2$	93.89	1.56	2.28 [44]	2.312

[a] ANTA/Kel-F 800 (95/5) ; [b] Explosive D/HTPB/BDNPA-F/MDI (80/12/6.5/1.5)

For the DINGU/HNE/wax formulation, the reported experimental $\Delta_f H^0$ value of -47 kJ/mol is less negative than the value of -95.1 kJ/mol calculated from the enthalpy of formation of -344 kJ/mol reported for DINGU in the ICT database (Table S3). However, as illustrated in Fig.4 of the article, this makes little difference regarding the calculated Gurney velocity of the composition.

Similarly, for NTO, in addition to the value of -100.7 kJ/mol suggested by the reviewer (Table S3), a more negative value of -129.4 kJ/mol is reported in the NIST Chemistry Webbook (https://webbook.nist.gov). Again, it is clear from Fig. 4 that this causes only a moderate decrease of the calculated Gurney velocity for pure NTO and for the NTO/HNE/wax formulation.

Table S3. Individual species and corresponding formation enthalpies used to estimate Gurney velocities reported in Table S2. For wax, the stoichiometry was approximated as simply CH_2 and the formation enthalpy as -29 kJ/mol per CH_2 unit. 1,2-DP do not enter the compositions reported in Table S2. There are included in this Table to demonstrate the structural diversity of present compounds.

DNAN (2,4-dinitroanisole)  -186.65 kJ/mol	SK TNBI  -414 kJ/mol	TNBI.2H$_2$O  -115 kJ/mol
Explosive D (Dunnite)  −385.44 kJ/mol [a]	ANTA  61.1 kJ/mol [b]	DINGU  -344 kJ/mol [c]
NITRA  93.89 kJ/mol	NTO  -100.7 kJ/mol	HNE  80.3 kJ/mol [d]

[a] A. Finch et al. *Thermochimica Acta*, 49, 281-285 (1981)

[b] R. L. Simpson et al. *IPropellants, Explos. Pyrotech. 19*, 174-176 (1994)

[c] H. Bathelt et al. *ICT Database of Thermochemical Values*, 7th Update (2004)

[d] M. A. Suntsova et al. *J. Chem. Eng. Data 59*, 2813-2826 (2013)