

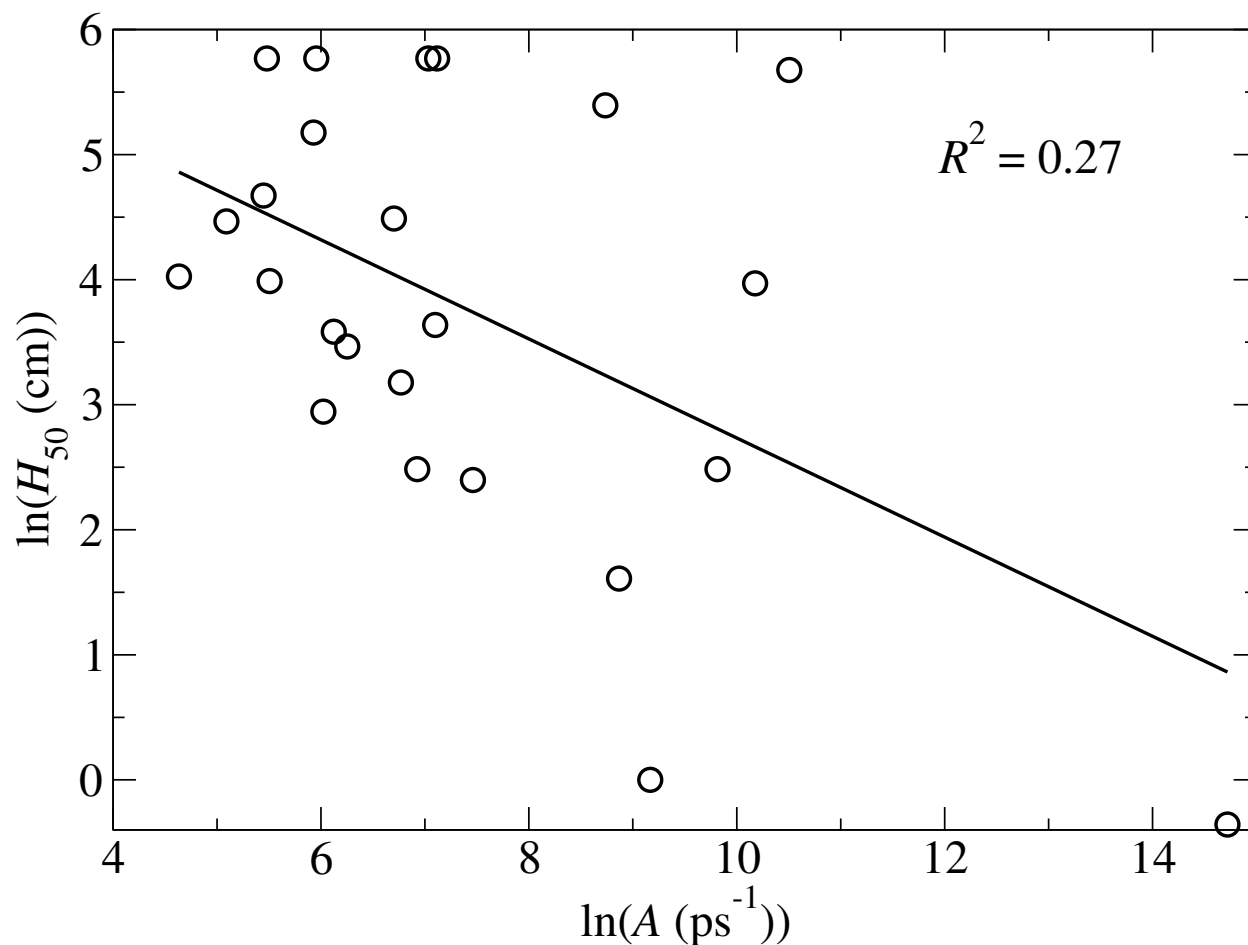
**Supplementary Material**  
**Understanding explosive sensitivity with effective trigger linkage kinetics**

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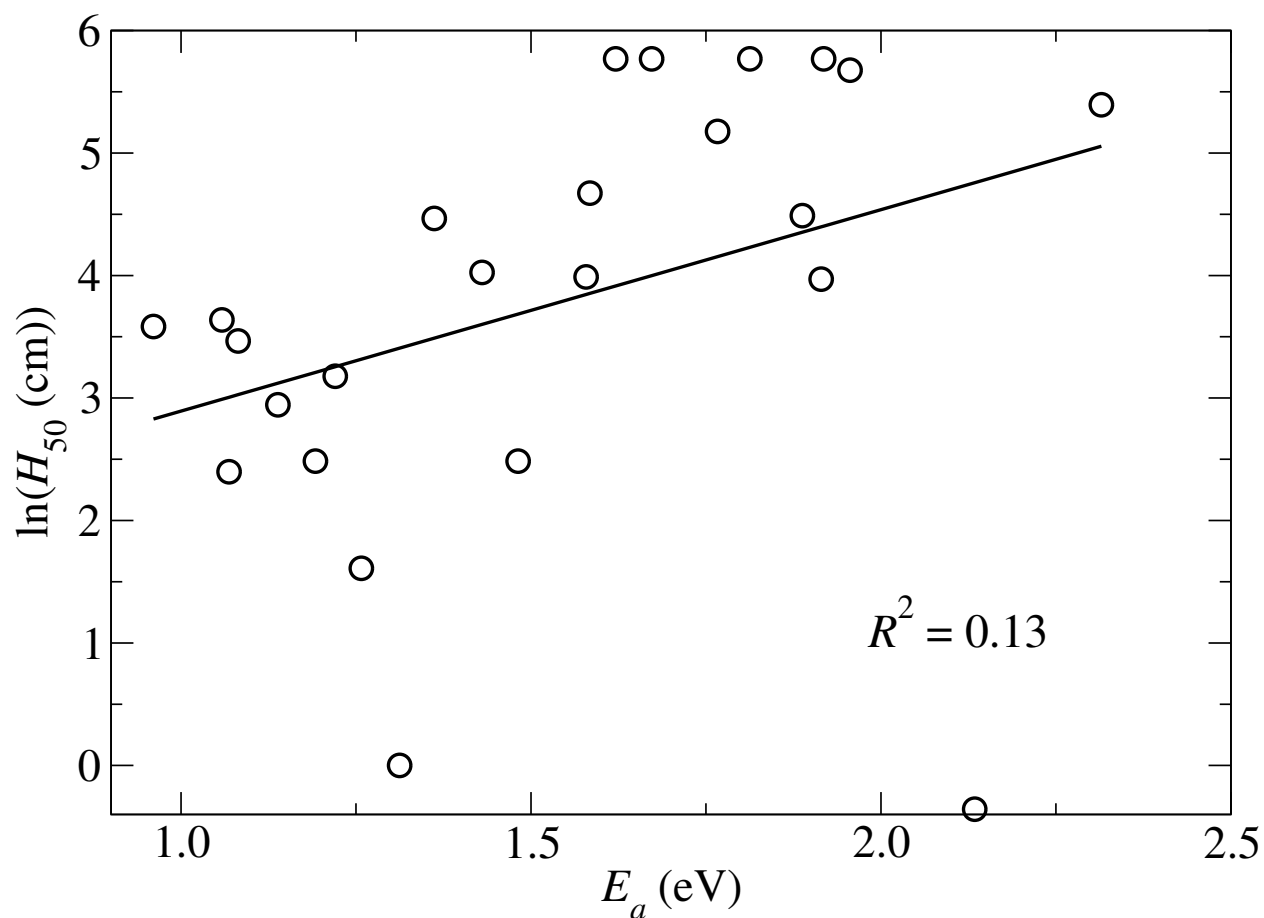
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**1. Correlations between  $H_{50}$  and Arrhenius rate pre-factors and activation energies.**



**Figure S1:** Dependence of  $\ln(H_{50})$  on  $\ln(A)$  obtained from the rates of trigger linkage rupture. The solid line represents the linear regression to the data.



**Figure S2:** Dependence of  $\ln(H_{50})$  on the activation enthalpy,  $E_a$ , obtained from the rates of trigger linkage rupture. The solid line represents the linear regression to the data.

## 2. Comparison of drop weight impact sensitivities

**Table S1.** The drop weight impact sensitivities calculated from the model (Eq. 14,  $R^2 = 0.71$ ) and experimental data.

Molecule	Model $H_{50}$ (cm)	Experiment $H_{50}$ (cm)
DAAF	23	292
ETN	6	5
HMX	19	32
NQ	129	320
PETN	7	12
PETNCH	20	24
PETNCMe	27	12
PETNCNH <sub>2</sub>	16	36
RDX	26	19
TATB	184	320
TNA	234	177

ETNA	31	53
Tetryl	17	38
2,3,4-TNT	137	56
3,4,5-TNT	138	107
2,4,6-TNT	203	220
DATB	220	320
Picric acid	162	87
LETN	6	1
ETA	3	0.7
CL-20	6	11
HNS	158	54
DNAN	203	320
TNBAL	245	89

### 3. Synthesis and drop weight testing of TNBAL

The value of the drop weight impact sensitivity of trinitrobenzene aldehyde (TNBAL) reported by Kamlet and Adolph [1] was found to be unexpectedly small,  $H_{50} = 36$  cm, based on the trigger linkage hypothesis developed in our manuscript. A new TNBAL sample was synthesized at LANL to reevaluate the published impact sensitivity. Drop weight impact testing (Type 12 tool, 2.5 kg mass) performed at LANL on the new TNBAL samples gave  $H_{50} = 89$  cm.

TNBAL was synthesized according to a two-step modified literature procedure [2, 3]. Recrystallized trinitrotoluene (TNT) (1500mg) and N,N-dimethyl-p-nitrosoaniline (1091mg) were suspended in 2.25 mL of pyridine. A few (10-15) crystals of  $I_2$  were added and the suspension was stirred for 7 days at room temperature. The black solution was filtered, washed with cold acetone and dried to yield 1.8g of black solid (76% yield). The black solid (744 mg) was then suspended in 6 mL of concentrated HCl and stirred for 3 hours at 60°C. The resulting red/black suspension was filtered, washed first with cold deionized water, then with a 1:1 mixture of dichloromethane/hexane and dried under vacuum to yield 520 mg of black, crystalline TNBAL.  $^1H$  NMR ( $CDCl_3$ , 400MHz):  $\delta$  10.64 (s, 1H, CHO),  $\delta$  9.30 (s, 2H, Aryl) DSC:

Impact testing was performed with LANL type 12 drop hammer equipment using a 2.5 kg weight according to literature methods [4, 5]. IS: 89 cm<sup>-1</sup>, 21.8 J.

### References

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