1   Supplementary Material

2   1. The relationship between the phonon-vibron coupling coefficients and impact

3   sensitivity based on the classification criteria.

4   Considering that molecular structure influences the impact sensitivity of energetic

5   materials, based on the classification criteria in Figure S1 (according to molecular

6   symmetry, types of functional groups, etc.), these 45 energetic explosives were divided

7   into two groups: the group A comprises 30 energetic molecules, and the group B

8   consists of 15 energetic molecules. Firstly, energetic materials are classified into two

9   broad categories depending on whether they include the ring structures. For energetic

10   materials with the ring structures, they are subdivided into groups based on the other

11   rings and the benzene rings. For energetic materials that do not contain the benzene

12   ring, compounds with triazinane are classified as group B, while compounds containing

13   cyclohexane or a five-membered heterocycle are classified as group A. Those with the

14   benzene rings are further divided based on whether they contain additional types of

15   rings. Energetic materials with the benzene rings and other types of rings are assigned

16   to group A if they include triazole or pyridine, and to group B if they include pyrazole.

17   For energetic materials with the benzene rings but no other types of rings, those lacking

18   the center symmetry are categorized into group A, and those with a center symmetry

19   into group B. For energetic materials without the ring structure, they are categorized

20   into two groups based on the specific types of functional groups contained in their

21   molecules. Those with nitro groups connected by oxygen or nitrogen ($O-NO_2$ or $N-$

22   NO_2) belong to one group, while those with nitro groups connected only by carbon ($C-$

23   NO_2) fall into another group. Among the energetic materials with nitro groups linked

24   by oxygen or nitrogen ($O-NO_2$ or $N-NO_2$), those with a molecular structure that is

25   centrally symmetric are placed in group B, and those with a non-centrally symmetric

26   molecular structure are placed in group A. Compounds with nitro groups connected

27   solely by carbon ($C-NO_2$) are further divided into three groups based on the number of

28   carbon atoms in the molecule. Compounds with 1 to 3 carbon atoms constitute one

29   group, those with 4 to 7 carbon atoms another group, and those with exactly 8 carbon

30 atoms form a third group. For energetic materials with 1 to 3 carbon atoms, those

31 containing the -CH$_3$ (methyl) functional group are assigned to group A, while those

32 with the -OH (hydroxyl) functional group are assigned to group B. For energetic

33 materials with 4 to 7 carbon atoms, if the ratio (the number of nitro groups on carbon

34 atoms connected to nitro groups compared to the sum of -CH$_3$ and -CH$_2$ (methyl and

35 methylene) groups) is less than 1, these materials are categorized into group A; if the

36 ratio is equal to 1, they are categorized into group B. For energetic materials with 8

37 carbon atoms, if each carbon atom connected to a nitro group is also connected to at

38 least two nitro groups, then these materials belong to group A. If each carbon atom

39 connected to a nitro group is attached to fewer than two nitro groups, then these

40 materials are classified into group B. "N$_{NO2}$" denotes the number of nitro groups. Their

41 molecular structures and chemical formulas are illustrated in Figure S2 (group A) and

42 Figure S3 (group B). The chemical name, molecular formula, isomeric SMILES,

43 phonon-vibron coupling coefficients ($\zeta \times 10^4$) and impact sensitivity (H$_{50}$) of group A

44 and group B energetic materials are shown in

45 Table S4 and Table S5. The computed frequencies (cm^{-1}) in 0-700cm^{-1} for group A and

46 group B energetic materials are shown in Table S6 and Table S7.

47　　Different functional relationships are provided for the dependency between coupling

48 factors and impact sensitivity for the two groups of energetic molecules. The obtained

49 |R| values are depicted in the histograms of a two-dimensional array in Figures S4(a)

50 and (b). As displayed in Figure S5 (a) and (b), both coupling coefficients and impact

51 sensitivity exhibit a high correlation. For the group A energetic materials, the

52 correlation coefficient is 0.88, and for the group B, the correlation coefficient is 0.89.

53 This also reaffirms the need to consider the impact of chemical structure when studying

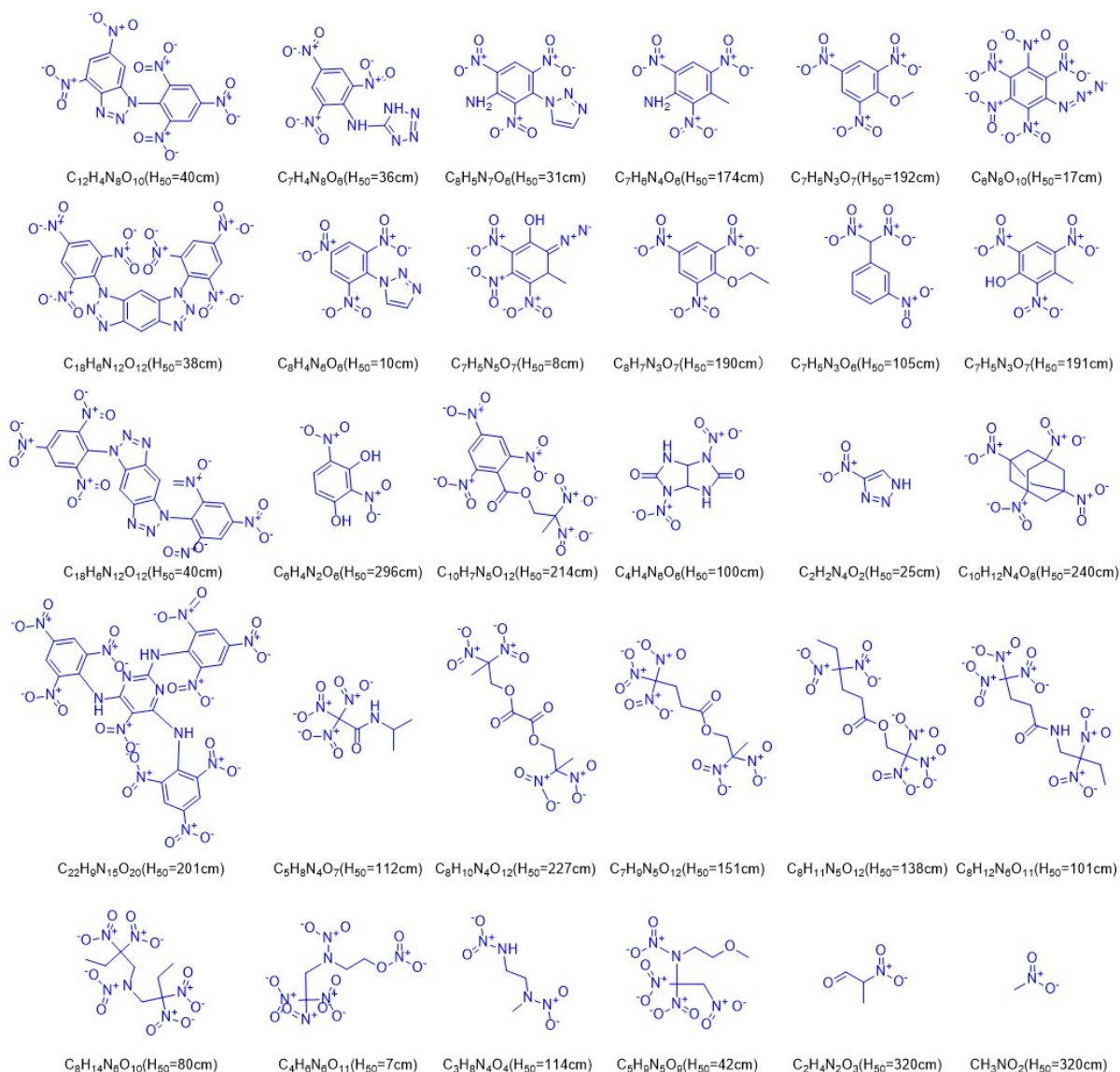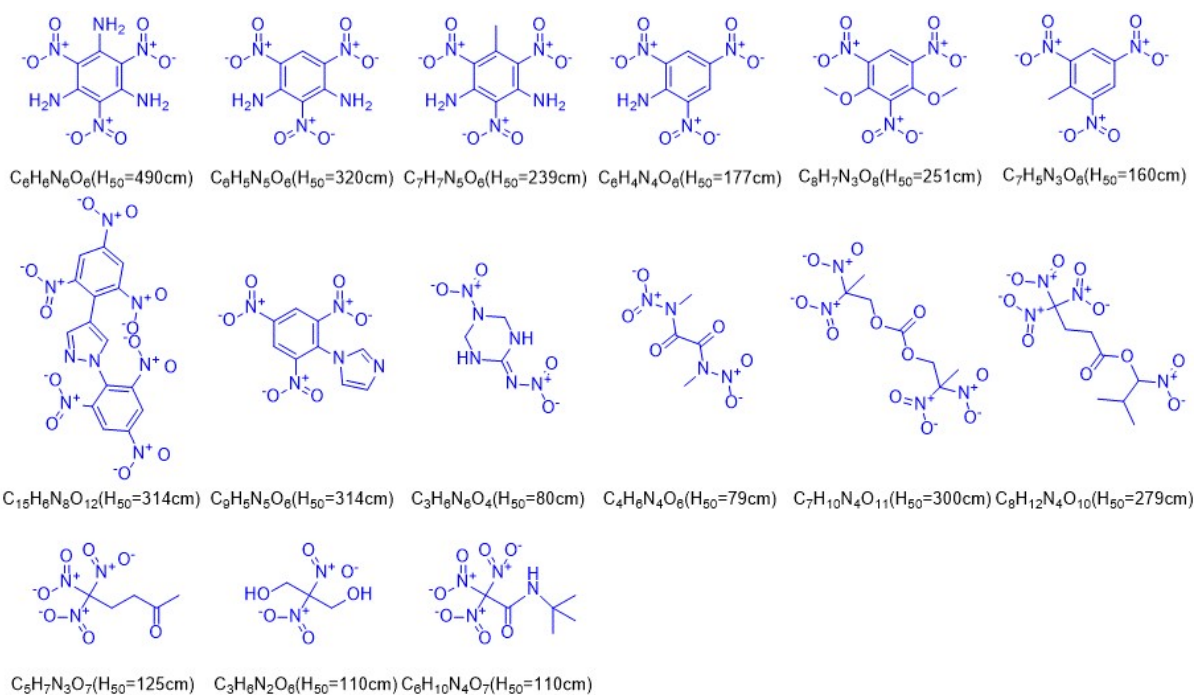54 the impact sensitivity of energetic materials.

55

56

57

58
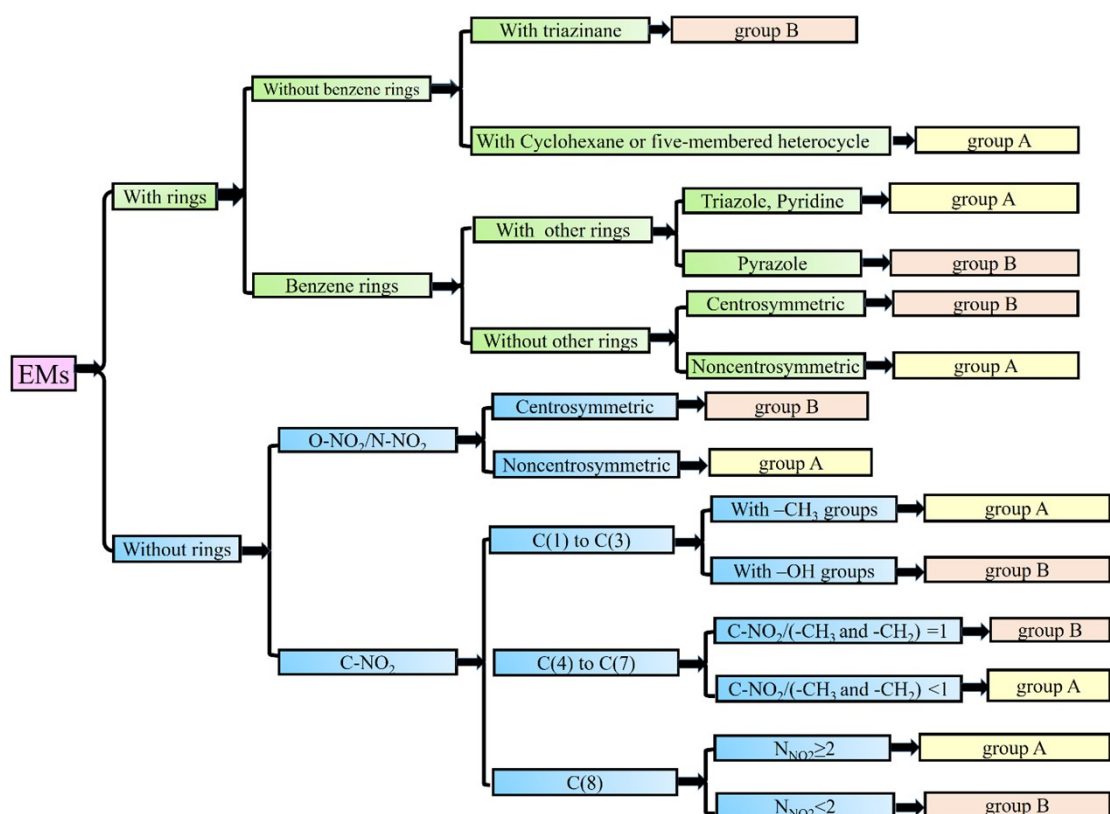
59 Figure S1. Classify energetic materials based on features such as structure, symmetry,

60 number of carbon atoms, and functional groups.

61
62
63
64
65
66
67
68
69
70
71
72
73
74
75
76
77

$C_{12}H_4N_8O_{10}(H_{50}=40cm)$ $C_7H_4N_8O_8(H_{50}=36cm)$ $C_8H_5N_7O_6(H_{50}=31cm)$ $C_7H_6N_4O_6(H_{50}=174cm)$ $C_7H_5N_3O_7(H_{50}=192cm)$ $C_8N_8O_{10}(H_{50}=17cm)$

$C_{18}H_6N_{12}O_{12}(H_{50}=38cm)$ $C_8H_4N_8O_6(H_{50}=10cm)$ $C_7H_5N_5O_7(H_{50}=8cm)$ $C_8H_7N_3O_7(H_{50}=190cm)$ $C_7H_5N_3O_6(H_{50}=105cm)$ $C_7H_5N_3O_7(H_{50}=191cm)$

$C_{18}H_6N_{12}O_{12}(H_{50}=40cm)$ $C_6H_4N_2O_6(H_{50}=296cm)$ $C_{10}H_7N_5O_{12}(H_{50}=214cm)$ $C_4H_4N_6O_6(H_{50}=100cm)$ $C_2H_2N_4O_2(H_{50}=25cm)$ $C_{10}H_{12}N_4O_8(H_{50}=240cm)$

$C_{22}H_9N_{15}O_{20}(H_{50}=201cm)$ $C_5H_8N_4O_7(H_{50}=112cm)$ $C_8H_{10}N_4O_{12}(H_{50}=227cm)$ $C_7H_9N_5O_{12}(H_{50}=151cm)$ $C_8H_{11}N_5O_{12}(H_{50}=138cm)$ $C_8H_{12}N_6O_{11}(H_{50}=101cm)$

$C_8H_{14}N_6O_{10}(H_{50}=80cm)$ $C_4H_6N_6O_{11}(H_{50}=7cm)$ $C_3H_8N_4O_4(H_{50}=114cm)$ $C_5H_9N_5O_9(H_{50}=42cm)$ $C_2H_4N_2O_3(H_{50}=320cm)$ $CH_3NO_2(H_{50}=320cm)$

78 Figure S2. The molecular structures, molecular formulas, and impact sensitivity (H_{50})
79 of group A energetic materials.
80
81
82
83
84
85
86
87
88
89
90
91
92

C₆H₆N₆O₆(H₅₀=490cm) C₆H₅N₅O₆(H₅₀=320cm) C₇H₇N₅O₆(H₅₀=239cm) C₆H₄N₄O₆(H₅₀=177cm) C₈H₇N₃O₈(H₅₀=251cm) C₇H₅N₃O₆(H₅₀=160cm)

C₁₅H₆N₈O₁₂(H₅₀=314cm) C₉H₅N₅O₆(H₅₀=314cm) C₃H₆N₆O₄(H₅₀=80cm) C₄H₆N₄O₆(H₅₀=79cm) C₇H₁₀N₄O₁₁(H₅₀=300cm) C₈H₁₂N₄O₁₀(H₅₀=279cm)

C₅H₇N₃O₇(H₅₀=125cm) C₃H₆N₂O₆(H₅₀=110cm) C₆H₁₀N₄O₇(H₅₀=110cm)

93 Figure S3. The molecular structures, molecular formulas, and impact sensitivity values
94 of group B energetic materials.
95
96
97
98
99
100
101
102
103
104
105
106
107
108
109
110
111
112
113
114
115
116
117
118
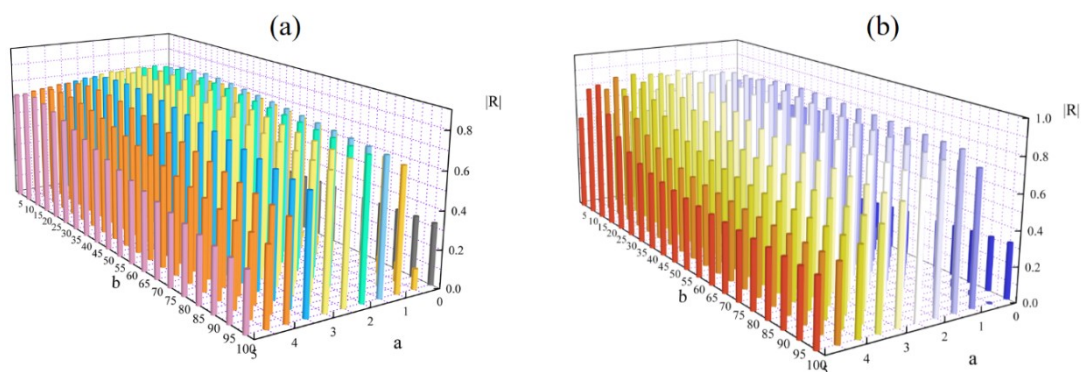
Figure S4. (a) The relationship between |R| and both damping factors a and b for the first set of energetic materials; (b) The relationship between |R| and both damping factors a and b for the second set of energetic materials.
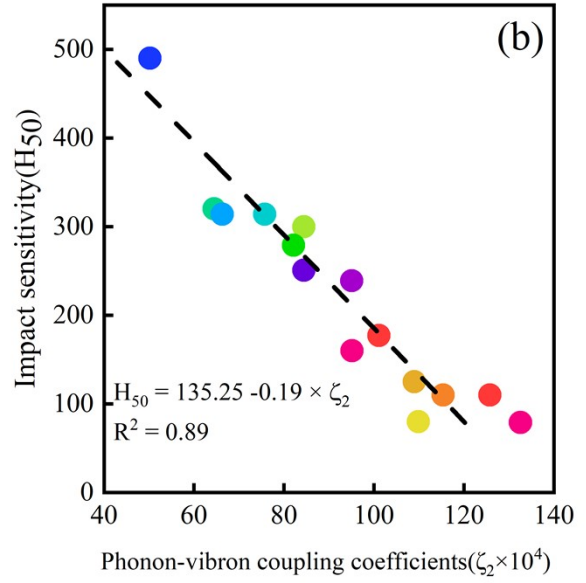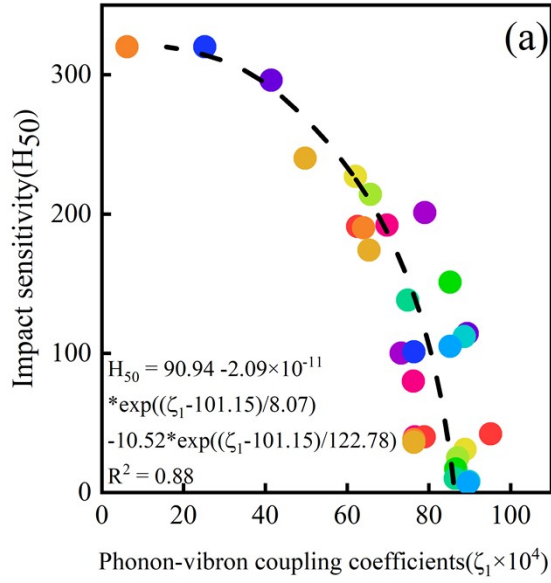
Figure S5. (a) The relationship between ζ_1 and impact sensitivity H_{50} for the first set of energetic materials; (b) The relationship between ζ_2 and impact sensitivity H_{50} for the second set of energetic materials.