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REGULAR ARTICLE

An evaluation of nitro derivatives of cubane using ab initio and density functional theories

Jinshan Li

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Abstract A novel method for judging the energy output of energetic compounds has been deduced from the conservation of energy condition. On the basis of B3LYP/6-31++G** fully optimized geometries, the enthalpy of formation, crystal density, detonation velocity and pressure for polynitrocubanes have been calculated using various theoretical methods. It has been observed that for polynitrocubanes the introduction of $–NH_2$ group onto the skeleton results in the destabilization of the neighboring C–C bonds on the skeleton. The C–C and $C–NO_2$ bonds of octanitrocubane (ONC) are stronger than those of partly nitrated cubanes, implying that the shock stability of ONC is superior to that of partly nitrated cubanes. For polynitrocubanes the calculated crystal density by the Karfunkel–Gdanitz ab initio method is within 0.07 g/cm^3 of experimental crystal density, being more accurate than by the group additivity method. The detonation velocity, the detonation pressure, and the energy output all increase from tetranitrocubane to ONC. The detonation velocity and pressure of ONC are predicted to reach 9.58 km s^{-1} and 60.0 Gpa, respectively. It is first indicated that the energy output for 1, 2, 3, 5, 8-pentanitrocuban is close to that of the widely used high explosive HMX and for ONC is about 80% larger than that of HMX.

Keywords High-energy compound · Polynitrocubane · Energy output · Ab initio method

1 Introduction

Energetic compounds are widely used in various fields. There is an ongoing need for high-energy compounds. In order to look for powerful, shock-insensitive, high-density compounds, polynitrocubanes have received worldwide attention [1]. Over the past 20 years, Eaton and co-workers have synthesized a series of nitro derivatives [2–5], and have found a novel species of energetic compounds. Although cubane has large strain energy, polynitrocubanes are thermally stable with decomposition points above 200 °C. In addition, the experiments with diamond anvil high pressure cells (DAC) reinforced that the nitro groups on the cubane skeleton, while conferring more explosive power to the compound, at the same time make it less sensitive to such external stimuli as heat and high stresses [6]. Unfortunately, the experimental data for the sensitivity and performance of polynitrocubanes are not reported nowadays, which determine their practical values. Consequently it is significant to predict theoretically the properties of polynitrocubanes. Although there have been some theoretical studies on other polynitrocubanes to date [7–12], the property of energy output of polynitrocubanes remains to be settled, which is the most important of detonation performances for energetic compounds.

In order to evaluate polynitrocubanes, this work systematically investigates a series of nitro derivatives of cubane. Firstly, a novel method for judging the energy output of energetic compound has been developed from the conservation of energy condition. Then the properties of enthalpy of formation, crystal density, and detonation performance for polynitrocubanes are investigated from ab initio calculations, and particularly the energy output for polynitrocubanes has been evaluated. Obviously this work

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J. Li (✉)
Institute of Chemical Materials,
China Academy of Engineering Physics,
621900 Mianyang, Sichuan,
People's Republic of China
e-mail: ljs915@263.net

sheds some light on the theoretical design of energetic compounds at the ab initio level.

2 Computational methods and details

2.1 Molecular and crystal structures

The quantum chemical calculations have been carried out employing the GAUSSIAN 03 W program [13]. In order to investigate systematically, the polynitrocubanes studied here are 1, 4-dinitrocubane (DNC), 1, 3, 5-trinitrocubane (TriNC), 1, 3, 5, 7-tetranitrocubane (TNC), 1, 2, 3, 5, 8-pentanitrocubane (PNC), 1, 2, 3, 4, 5, 7-hexanitrocubane (HNC), 1, 2, 3, 4, 5, 6, 8-heptanitrocubane (HpNC), and octanitrocubane (ONC). It is well-known that the introduction of –NH_2 group into 1, 3, 5-trinitrobenzene can get less sensitive molecules. So the aminonitrocubane compound 1, 4-diamino-2, 3, 5, 6, 7, 8-hexanitrocubane (DAHNC) has also been studied to discuss the influence of –NH_2 group on the stability of polynitrocubanes. Figure 1 displays the atomic numberings of polynitrocubane skeleton, which is consistent with the positions of above substituents. The density functional B3LYP method [14] and the 6–31++G** basis set have been used to optimize all molecular structures without any symmetry restriction and to analyze vibrational frequency. The natural bond orbital analysis [15] has been carried out at the level of MP2/6-31++G**//B3LYP/6-31++G**.

The ab initio crystal structure prediction method proposed by Karfunkel and Gdanitz [16] (hereafter called the Karfunkel–Gdanitz method) contained in the Materials Studio software [17] has been employed to predict the crystal density from molecular structure, which proves to be feasible in our previous study [18]. During the ab initio prediction of crystal structure, the Dreiding force field [19], which models carbon, nitrogen, oxygen, and hydrogen accurately, has been adopted, and the 17 most common space groups are considered [20].

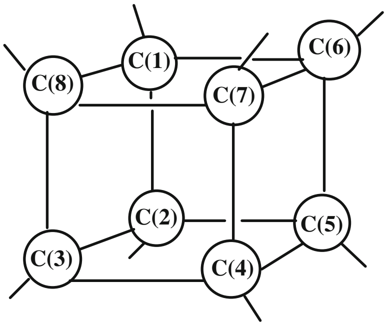

Fig. 1 Atomic numberings for polynitrocubane skeleton

2.2 Detonation performance

For a detonation wave propagating with velocity D into an energetic material initially at rest, the conservation of energy condition is [21]

$$E_1 - E_0 = \frac{1}{2}(P_1 + P_0)(V_0 - V_1) + Q \tag{1}$$

where E_0, P_0, and V_0 are, respectively, the internal energy of the solid explosive per unit mass, pressure, and specific volume, E_1, P_1, and V_1 are, respectively, the final internal energy per unit mass, pressure, and specific volume, and Q is the specific chemical energy released by the detonation of energetic compound. Considering $P_1 \gg P_0$ Eq. 1 can be written as

$$E_1 - E_0 = \frac{1}{2}P_1(V_0 - V_1) + Q \tag{2}$$

If the detonation products are regarded as polytropic gases $P = \mathrm{B}V^{-k}$ where k is the polytropic exponent, the detonation pressure (P_{CJ}) and the specific volume (V_{CJ}) at the Chapman-Jouguet (C-J) point can be expressed as [21]

$$P_{\mathrm{CJ}} = \frac{1}{k+1}\rho_0 D^2 \tag{3}$$

$$V_{\mathrm{CJ}} = \frac{k}{k+1}V_0 \tag{4}$$

$$D = \sqrt{2(k^2-1)Q} \tag{5}$$

where ρ_0 is the initial density. Substituting Eqs. 3–5 into Eq. 2 yields the energy release per unit mass at the C-J point

$$E_{\mathrm{CJ}} - E_0 = \frac{k}{k-1}\frac{D^2}{(k+1)^2} = \frac{(\rho_0 D^2 - P_{\mathrm{CJ}})P_{\mathrm{CJ}}^2}{(\rho_0 D^2 - 2P_{\mathrm{CJ}})\rho_0^2 D^2} \tag{6}$$

Obviously the value of $E_{\mathrm{CJ}} - E_0$ can reflect the driving force of detonation products. Based on the crystal density and the solid phase enthalpy of formation, the VLW equation of state (EOS) method [22] has been used to calculate the detonation velocity and pressure. In order to confirm the reliability of VLW method, the detonation velocity has also been calculated using the convenient Stine method [23]

$$D = 3.69 + \rho_0[13.85n_{\mathrm{C}} + 37.74n_{\mathrm{N}} + 68.11n_{\mathrm{O}} + 3.95n_{\mathrm{H}} + 0.1653\Delta H_{\mathrm{f}}^0(\mathrm{s})]/M \tag{7}$$

where D is in km s^{-1}, ρ_0 is in g cm^{-3}, $\Delta H_{\mathrm{f}}^0(\mathrm{s})$ is the solid phase enthalpy of formation at $T = 298.2$ K and $P = 1$ atm and in kJ mol^{-1}, n_{C}, n_{N}, n_{O} and n_{H} are, respectively, the numbers of atoms C, N, O, and H, and M is the molecular mass of the compound. In general, the Stine method is more accurate than the famous Kamlet–Jacobs method [24] for CHNO energetic compounds.

3 Results and discussion

3.1 Geometry and bond order

Molecular structure has important influence on susceptibility to shock- and impact-induced reactivity [25–27]. In fact, for most nitroaromatic compounds it has been confirmed that the C–NO_2 bond is of key importance in determining impact and shock sensitivities [28–30]. The stronger the C–NO_2 bond, the less sensitive the compound. But for polynitrocubanes it is realistically postulated that both C–C and C–NO_2 bonds would be related to impact and shock sensitivities.

Vibrational analysis shows there are no imaginary frequencies for all optimized structures at this theoretical level, which suggests that all the structures obtained are local minima on the potential energy surface. Table 1 gives the calculated longest bond length and the least bond order for C–C and C–NO_2 bonds. Generally the C–C bond is stronger than the C–N bond. However, for polynitrocubanes, the least bond order of C–C bond is smaller than that of C–NO_2 bond, this is ascribed to the existence of large cage strain effect. That is to say, for polynitrocubanes the weakest C–C bond breaks more easily under shock and impact stimulations. Compared with that of cubane, for partly nitrated cubanes the longest C–C bond lengthens slightly, but for fully nitrated cubane (ONC) it shortens. It is strange that the least bond orders of both C–C and C–NO_2 bonds of ONC are larger than the corresponding values of partly nitrated cubane.

Table 1 The longest bond length (r) and the least bond order (η) for C–C and C–NO_2 bonds of C_8H_8 and its nitro derivatives

Compounds	Parameters	
Cubane	$r_{1\text{–}2}$	1.571
	$\eta_{1\text{–}2}$	0.787
DNC	$r_{1\text{–}2}$	1.575
	$\eta_{6\text{–}7}$	0.777
	$r_{4\text{-NO2}}$	1.469
	$\eta_{4\text{-NO2}}$	0.813
TNC	$r_{1\text{–}8}$	1.577
	$\eta_{1\text{–}8}$	0.787
	$r_{3\text{-NO2}}$	1.475
	$\eta_{3\text{-NO2}}$	0.807
HNC	$r_{6\text{–}7}$	1.574
	$\eta_{6\text{–}7}$	0.786
	$r_{3\text{-NO2}}$	1.483
	$\eta_{3\text{-NO2}}$	0.803
ONC	$r_{2\text{–}3}$	1.570
	$\eta_{1\text{–}6}$	0.810
	$r_{3\text{-NO2}}$	1.486
	$\eta_{2\text{-NO2}}$	0.856
DAHNC	$r_{1\text{–}8}$	1.650
	$\eta_{1\text{–}8}$	0.735
	$r_{5\text{-NO2}}$	1.479
	$\eta_{7\text{-NO2}}$	0.814

See Fig. 1 for atomic numbering. r in Å

For aromatics and other unsaturated systems, the proper introduction of –NH_2 group can usually get a stable and insensitive molecule. However, for DAHNC the –NH_2 group makes the neighboring bond $r_{1\text{–}8}$ lengthen to 1.650 Å and the corresponding bond order decreases significantly, which is in agreement with the destabilizing effect of adjacent nitro and amino groups concluded by the previous ab initio study [31]. Accordingly for polynitrocubanes it is inappropriate to introduce the –NH_2 group onto the skeleton.

3.2 Gas phase enthalpy of formation

For energetic compounds the gas phase enthalpy of formation is an important thermodynamic property. The experimental value of gas phase enthalpy of formation [$\Delta H_f^0(g)$] at $T = 298.2$ K and $P = 1$ atm for reference compounds CH_4, CH_3NH_2, CH_3NO_2, and C_8H_8 is given in Table 2. In order to calculate the gas phase enthalpy of formation of polynitrocubane, the isodesmic concept has been adopted. The designed isodesmic reaction that preserves the integral cubane frame is

$$C_8H_{8-x-y}(NO_2)_x(NH_2)_y + (x+y)CH_4 \rightarrow C_8H_8 + xCH_3NO_2 + yCH_3NH_2 \qquad (8)$$

where x and y stand for the numbers of –NO_2 and –NH_2 groups, respectively. By employing the isodesmic reaction, the B3LYP/6-31++G** calculated value of enthalpy (H^0) at $T = 298.2$ K and $P = 1$ atm for reactants and products, which is corrected for the zero point energy (ZPE), and the above experimental $\Delta H_f^0(g)$ value for reference compounds, the calculated $\Delta H_f^0(g)$ for polynitrocubanes is listed in Table 3. Obviously the nitro derivatives of cubane

Table 2 Experimental gas phase enthalpy of formation and B3LYP/6-31++G** calculated total energy (E), zero point energy, and enthalpy for reference compounds

Compounds	$\Delta H_f^0(g)^{exp}$ (kJ mol^{-1})	E^a (hartree)	ZPE (kJ mol^{-1})	H^{0a} (hartree)
CH_4	-74.8^b	−40.5261512	117.6	−40.477560
CH_3NH_2	-23.0^b	−95.8719773	168.1	−95.803596
CH_3NO_2	-81.1^c	245.0288033	130.8	−244.973673
C_8H_8	622.2^d	−309.4799465	350.4	−309.340995

[a] H^0 is corrected for zero point energy and E is not

[b] From [32]

[c] From [33]

[d] From [34]

Table 3 B3LYP/6-31++G** calculated total energy, zero point energy, enthalpy, and gas phase enthalpy of formation for nitro derivatives of cubane

Compounds	E^{a} (hartree)	ZPE (kJ mol^{-1})	H^{0a} (hartree)	ΔH_f^0(g) (kJ mol^{-1})
DNC	−718.5037408	362.6	−718.355358	551.5
TriNC	−923.0053948	368.3	−922.851095	546.2
TNC	−1,127.5025086	373.2	−1,127.343409	549.8
PNC	−1,331.9855491	378.0	−1,331.821765	590.2
HNC	−1,536.46723	382.9	−1,536.298832	633.9
HpNC	−1,740.9442264	387.4	−1,740.771326	689.6
ONC	−1,945.4195212	391.8	−1,945.242141	749.7

[a] H^0 is corrected for zero point energy and E is not

Table 4 Calculated crystal density, binding energy, and lattice parameter (a, b, c, α, β, and γ) for typical polynitrocubanes

Compounds	ρ_{exp} (g cm^{-3})	ρ_{add} (g cm^{-3})	Space groups	ΔE (kJ mol^{-1})	ρ_{K-D} (g cm^{-3})	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
TNC	1.814	1.922	P-1	188.3	1.680	9.85	9.79	6.45	73.0	70.9	84.5
			$Pna2_1$	186.2	1.779	12.99	12.68	6.44	90.0	90.0	90.0
			$P2_1$	184.5	1.778	6.45	9.07	9.08	90.0	87.8	90.0
			$P2_12_12_1$	184.5	1.776	9.09	12.90	9.06	90.0	90.0	90.0
			Pbca	181.6	1.715	13.13	26.00	6.45	90.0	90.0	90.0
PNC	1.959	1.985	$P2_12_12_1$	192.5	1.843	13.14	6.79	13.30	90.0	90.0	90.0
			P-1	189.5	1.892	7.53	6.82	17.12	117.8	107.0	113.4
			P1	187.9	1.835	7.40	6.91	6.80	96.0	111.6	108.0
			Pbca	187.4	1.800	12.81	13.12	14.45	90.0	90.0	90.0
			$P2_1/c$	185.4	1.822	6.86	22.54	8.39	90.0	112.4	90.0
HNC	1.931	2.035	P-1	179.9	1.928	8.58	7.12	11.17	104.6	90.2	102.0
			$P2_1/c$	179.5	1.930	7.71	24.98	7.18	90.0	111.4	90.0
			C2/c	179.1	1.926	11.99	8.43	25.81	90.0	98.2	90.0
			$P2_12_12_1$	177.4	1.934	13.53	7.09	13.40	90.0	90.0	90.0
			$P2_1$	175.3	1.890	7.48	11.35	8.57	90.0	115.3	90.0
HpNC	2.028	2.077	$P2_12_12$	163.6	1.962	13.39	12.92	8.20	90.0	90.0	90.0
			Pbca	159.8	1.910	14.23	26.78	7.65	90.0	90.0	90.0
			P-1	156.1	1.906	8.82	7.39	14.47	99.1	119.1	107.7
			$Pca2_1$	155.6	1.941	13.90	7.84	13.16	90.0	90.0	90.0
			C2/c	155.2	1.870	27.30	7.66	14.27	90.0	85.2	90.0
ONC	1.979	2.111	P-1	147.3	2.065	7.63	14.97	7.63	65.6	70.6	85.9
			$P2_1$	134.7	1.954	8.60	12.26	7.58	90.0	99.3	90.0
			$P2_1/c$	131.0	1.971	7.59	28.66	7.59	90.0	108.8	90.0
			$Pna2_1$	129.7	1.932	15.29	12.26	8.51	90.0	90.0	90.0
			C2/c	128.0	1.930	14.43	15.26	14.73	90.0	99.7	90.0

have very large positive enthalpy of formation. For polynitrocubanes the ΔH_f^0(g) increases with the number of nitro groups increasing from 2 to 8, and for ONC it reaches 749.7 kJ mol^{-1}, which is in line with the previous value (726.5 kJ mol^{-1}) by Zhang and Xiao [9].

3.3 Crystal structure and detonation performance

Crystal density influences directly the detonation performance. The calculated crystal density (ρ_{K-D}), binding energy (ΔE), and lattice parameter by the Karfunkel–Gdanitz method are arranged in Table 4 for the five space groups with lower total energy. For convenient comparison Table 4 also gives the calculated crystal density (ρ_{add}) by the group additivity method [35] and the experimental value (ρ_{exp}). An energetic compound usually has several polymorphs, which can be obtained from recrystallization with different solvents, and we are interested in the polymorph with larger crystal density. It can be observed from Table 4 that generally the larger the binding energy, the higher the crystal density. For TNC, PNC, HNC, and HpNC, the changes of binding energy from the five space groups are within 8.5 kJ mol^{-1}, implying that for these compounds all the five polymorphs can appear possibly. But for ONC the value of ΔE (147.3 kJ/mol) with the P-1 space group is much larger than with other space groups, so the crystal structure with the P-1 space group may appear on the basis of thermochemical considerations alone.

A comparison between the values of $\rho_{\rm add}$ and $\rho_{\rm exp}$ in Table 4 shows that for TNC, HNC, and ONC the group additivity method overestimates the crystal density by over 0.1 g cm^{-3}, implying that one should be careful of the results from the group additivity method. The largest values of $\rho_{\rm K-D}$ for TNC, PNC, HNC, HpNC, and ONC are 1.779 (Pna2$_1$), 1.892 (P-1), 1.934 (P2$_1$2$_1$2$_1$), 1.962 (P2$_1$2$_1$2), and 2.065 (P-1) g cm^{-3}, respectively, being within 0.07 g cm^{-3} of the corresponding experimental. Thereby, for the prediction of crystal density of polynitrocubane the Karfunkel–Gdanitz method is more accurate than the group additivity method.

In order to calculate the detonation performance of energetic compounds, the solid phase enthalpy of formation is necessary. A procedure for converting gas to solid phase enthalpy of formation has been developed by Politzer et al. [36] on the basis of the calculated electrostatic potential on the molecular surface. In this work, $\Delta H_{\rm f}^0({\rm s}) = \Delta H_{\rm f}^0({\rm g}) - \Delta E$. Based on $\rho_{\rm K-D}$ and $\Delta H_{\rm f}^0({\rm s})$ the calculated detonation parameters by the VLW EOS method and the Stine method are summarized in Table 5. In order to evaluate the energy output of polynitrocubanes, the widely used high-energy compound HMX is recommended as a reference, and from Eq. 6 the relative energy output for other energetic compounds is judged by

$$I_{\rm e} = \frac{(\rho_0 D^2 - P_{\rm CJ})P_{\rm CJ}^2}{(\rho_0 D^2 - 2P_{\rm CJ})\rho_0^2 D^2} \Bigg/ \frac{\left(\rho_{\rm HMX} D_{\rm HMX}^2 - P_{\rm HMX}\right)P_{\rm HMX}^2}{\left(\rho_{\rm HMX} D_{\rm HMX}^2 - 2P_{\rm HMX}\right)\rho_{\rm HMX}^2 D_{\rm HMX}^2} \qquad (9)$$

where $P_{\rm HMX}$ is the experimental detonation pressure (39.3 GPa) for HMX, $D_{\rm HMX}$ is the detonation velocity (9.10 km s^{-1}), and $\rho_{\rm HMX}$ is the crystal density (1.906 g cm^{-3}). By using the calculated detonation parameters by the VLW EOS method, the calculated $I_{\rm e}$ for TNC, PNC, HNC, HpNC, and ONC is also listed in Table 5.

As far as the detonation velocities from the two methods are concerned, for TNC and PNC the calculated D by the VLW EOS method is 0.2–0.3 km s^{-1} larger than by the Stine method, and for HNC and HpNC is very close to that by the Stine method, but for ONC is 0.1–0.25 km s^{-1} less than by the Stine method, so the detonation velocities from the two methods are in good agreement. Table 5 tells that D, $P_{\rm CJ}$, and $I_{\rm e}$ all increase from TNC to ONC. The detonation velocity for HNC is close to that of HMX, but its detonation pressure surpasses that of HMX, resulting from its large enthalpy of formation and good oxygen balance. For ONC the values of D and $P_{\rm CJ}$ can arrive at 9.58 km s^{-1} and 60.0 Gpa, respectively, which are significantly higher than the corresponding values of HMX. The value of $I_{\rm e}$ for PNC approaches that of HMX, while for ONC it can be about 80% larger than that of HMX, implying that ONC is more powerful than compound CL-20, arguably the most powerful nonnuclear explosive known, whose energy output exceeds that of HMX by about 14% [37].

Table 5 Calculated solid phase enthalpy of formation, detonation velocity, detonation pressure, and relative energy output for typical polynitrocubanes

Compounds	Space groups	$\Delta H_{\rm f}^0$(s) (kJ mol^{-1})	Stine	VLW EOS		$I_{\rm e}$
			D (km s^{-1})	D (km s^{-1})	$P_{\rm CJ}$ (GPa)	
TNC	P-1	361.5	7.60	7.88	27.4	0.83
	Pna2$_1$	363.6	7.83	8.16	31.1	0.89
	P2$_1$	365.3	7.83	8.16	31.1	0.89
	P2$_1$2$_1$2$_1$	365.3	7.82	8.15	31.0	0.89
	Pbca	368.2	7.69	7.99	28.7	0.85
PNC	P2$_1$2$_1$2$_1$	397.7	8.38	8.62	37.8	1.10
	P-1	400.7	8.50	8.75	40.3	1.15
	P1	402.3	8.36	8.61	37.5	1.10
	Pbca	402.8	8.27	8.52	36.0	1.07
	P2$_1$/c	404.8	8.33	8.58	37.0	1.09
HNC	P-1	454.0	8.93	9.04	45.9	1.35
	P2$_1$/c	454.4	8.93	9.04	46.0	1.35
	C2/c	454.8	8.92	9.03	45.8	1.35
	P2$_1$2$_1$2$_1$	456.5	8.95	9.05	46.3	1.36
	P2$_1$	458.6	8.83	8.95	43.9	1.31
HpNC	P2$_1$2$_1$2	526.0	9.30	9.26	50.9	1.53
	Pbca	529.8	9.18	9.16	47.9	1.46
	P-1	533.5	9.14	9.15	47.7	1.46
	Pca2$_1$	534.0	9.24	9.22	49.7	1.50
	C2/c	533.4	9.04	9.07	45.8	1.42
ONC	P-1	602.4	9.83	9.58	60.0	1.79
	P2$_1$	615.0	9.51	9.37	52.8	1.62
	P2$_1$/c	618.7	9.57	9.41	53.8	1.64
	Pna2$_1$	620.0	9.45	9.33	51.5	1.59
	C2/c	621.7	9.45	9.33	51.4	1.59

4 Conclusions

This work has investigated the geometries, electronic structures, enthalpies of formation, crystal structures, and detonation parameters of polynitrocubanes. A novel method for evaluating the energy output of energetic compounds has been deduced from the conservation of energy condition. For polynitrocubanes the introduction of $-NH_2$ group onto the skeleton results in the destabilization of the neighboring C–C bonds on the skeleton. After full nitration both C–C and $C-NO_2$ bonds become stronger compared with those of partly nitrated cubanes, implying that the shock stability of ONC is superior to that of partly nitrated cubanes. For polynitrocubanes the calculated crystal density by the Karfunkel–Gdanitz ab initio method is more accurate than by the group additivity method. D, P_{CJ}, and I_e all increase from TNC to ONC. The detonation velocity and pressure for ONC can arrive at 9.58 km s^{-1} and 60.0 Gpa, respectively. It has been theoretically discovered that the energy output for 1, 2, 3, 5, 8-pentanitrocuban is close to that of HMX and for ONC is about 80% larger than that of HMX, indicating that highly nitrated cubanes are very powerful compounds.

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