



# Tetranitro-diazinodiazines as high energy materials: computational investigation of structural aspects of fused heterocyclic backbone and isomerism

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## Abstract

Thirteen tetranitro-diazinodiazines have been designed and investigated to find the importance of diazinodiazine fused-heterocyclic backbone for energetic materials. The positional influence of four nitrogen atoms in the diazinodiazine backbone on the heat of formation, performance, and stability has been investigated by density functional theory. It is observed that diazinodiazine is an efficient backbone to improve energy content in the designed derivatives. The energy contribution from the diazinodiazine backbone varies from 352–558 kJ/mol. Introducing four  $-\text{NO}_2$  groups into the diazinodiazine backbone resulted in new energetic molecules with acceptable detonation performance and stability. Their densities, detonation velocities, and detonation pressures were 1.87–1.89 g/cm<sup>3</sup>, 8.36–8.68 km/s, and 31.72–34.42 GPa, respectively. The bond dissociation energies for the longer C–NO<sub>2</sub> bonds fall in the range of 207–233 kJ/mol, reveals the stable nature of tetranitro-diazinodiazines. Thus, diazinodiazine isomers may be regarded as promising aromatic heterocyclic backbone, and tetranitro-diazinodiazines appear to be potential candidates for energetic materials.

**Keywords** Diazinodiazine, Energetic materials · Heat of formation · Detonation properties · Fused heterocycle

## Introduction

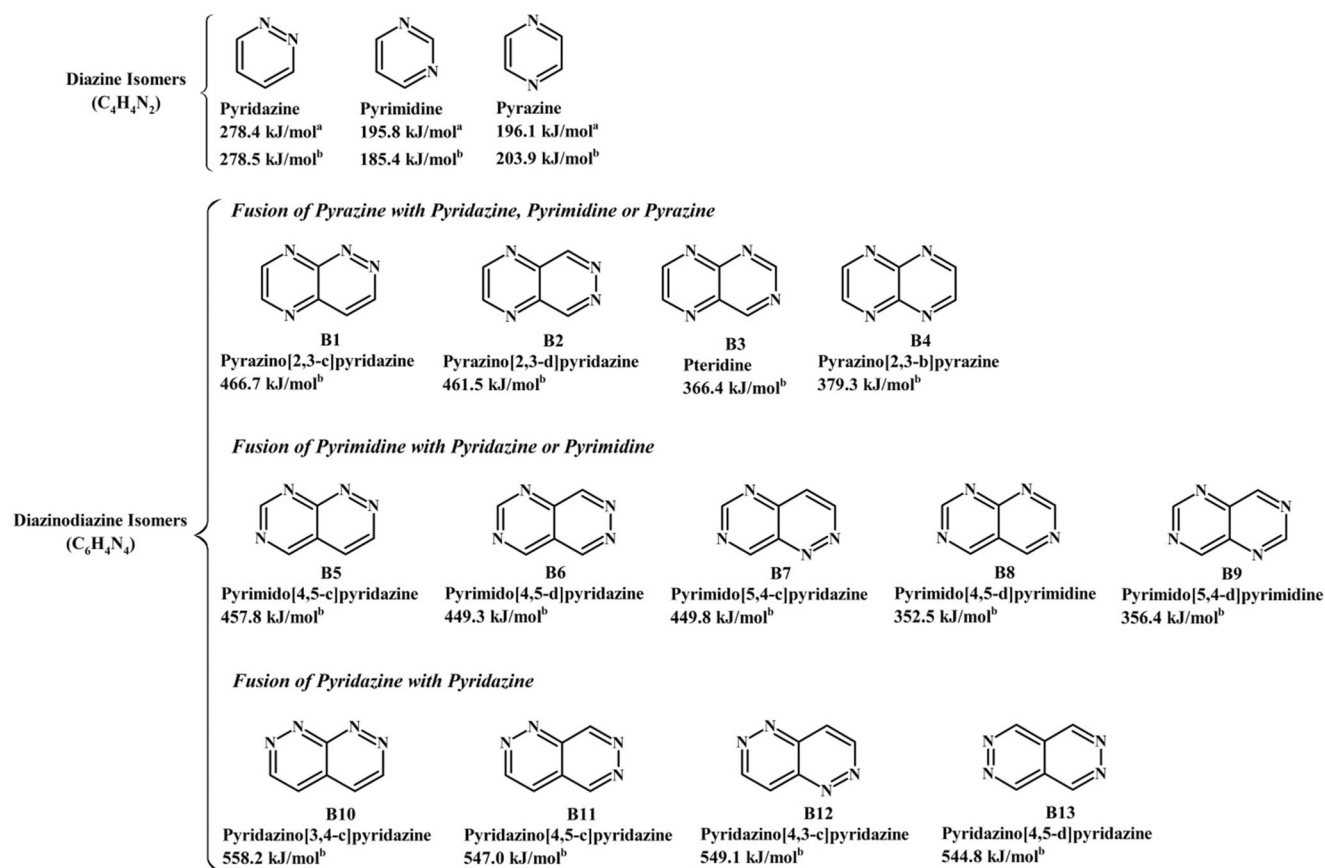
The search and development of new energetic materials that fulfill explicit requirements of high heat of formation (HOF), positive oxygen balance (OB), high crystal density, high detonation properties, and less sensitivity have attracted immense attention worldwide and a stubborn challenge for researchers. Considering the stringent requirement of performance and safety of explosives and propellants, in the past few decades, researchers' attention has drifted from benchmark nitramines, nitro esters, and nitroaromatic materials to nitrogen-rich heterocyclic compounds [1–10]. The introduction of nitrogen-rich heterocyclic backbone in energetic materials is proven

to be an excellent approach to improve the HOF, density, OB, and performance than their carbocyclic analogs [1, 2]. Furthermore, the high volume of nitrogen gas released in decomposition products exhibits the material's eco-friendly nature. Aromatic fused-heterocyclic rings are of great interest as energetic backbone owing to their high HOF and good thermal stability [2]. The current strategies to improve detonation performance involve introducing several nitro groups in the fused-heterocyclic rings, which would combine the advantages of each of the components in molecular structure. Here we scrutinize the diazinodiazines having fused six-membered diazine rings [11–14]. Replacement of the four methines ( $-\text{CH}=\text{}$ ) in naphthalene by nitrogen atoms gives diazinodiazine framework without altering the resulting rings aromatic behavior (see Fig. 1). The aromatic structure of diazinodiazines with four nitrogens can be a potential precursor and substrate for developing novel energetic materials. The nitro derivatives of diazinodiazines are less studied and less explored for their potential application in explosives. This work reports a computational study that reveals the significance of fused heterocyclic diazinodiazine backbone in designing energetic materials. We have introduced four  $-\text{NO}_2$  groups in the diazinodiazine backbone to improve the oxygen balance,

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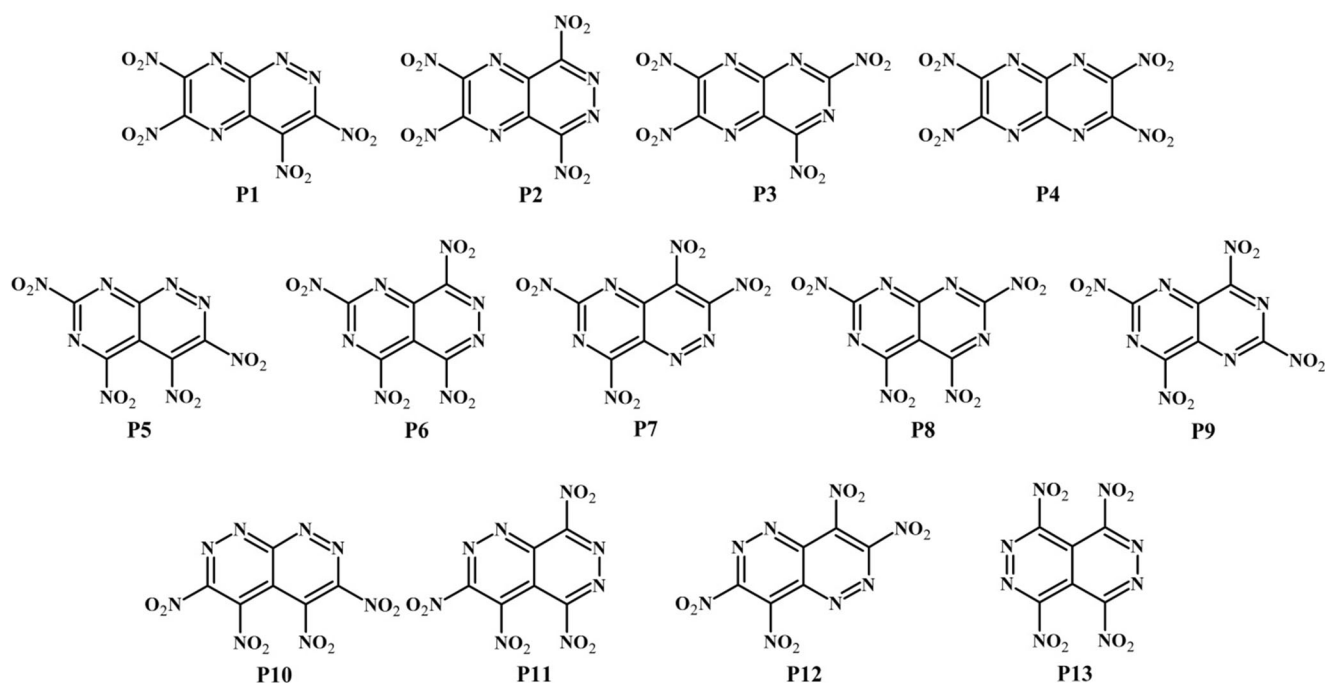
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**Fig. 1** Design idea for diazinodiazine derivatives. <sup>a</sup>Experimental gas phase HOF. <sup>b</sup>Calculated gas phase HOF using the G4 method

density, and performance and understanding the structure-performance-stability characteristics (see Fig. 2). We

envisioned that the arrangement of four nitrogens in the diazinodiazine framework and incorporation of  $-NO_2$  groups



**Fig. 2** Molecular structures of tetranitro-diazinodiazines ( $C_6N_8O_8$ )

offers opportunities for finding insensitive energetic materials with admirable performance properties.

## Computational method

Gaussian 09 program [15] was used to optimize the structures of tetranitro-diazinodiazines (Fig. 2) at B3PW91/6-31G(d,p) level. Optimized structures were confirmed as local energy minima on the potential energy surface without imaginary frequencies. The molecular surface analysis was carried out using the Multiwfn program [16]. The methods and equations adopted for the estimation of the energetic properties of the tetranitro-diazinodiazines are identical to our previous reports [17–19] and summarized in the [Supporting Information](#).

## Results and discussion

### Heat of formation

In energetic materials, HOF indicates the energy stored in the molecule. Compared to the single ring pyridazine, pyrimidine, and pyrazine frameworks, the fusion of these rings as diazinodiazine isomers possesses high positive HOFs due to a large number of C–N and N–N bonds (see Fig. 1). The HOF of diazinodiazine isomers was predicted using the Gaussian-4 (G4) theory [20, 21] and isodesmic reaction approach [22, 23] (see Figure S14). The  $HOF_{Gas}$  obtained from the G4 method are close to those computed from the isodesmic reaction approach. Prior studies also showed that the HOF values calculated with the G4 method are reliable and comparable to experimental values

[23–25]. Tables 1 and 2 summarize the calculated thermochemistry values and energy content for the diazinodiazine isomers and tetranitro-diazinodiazines, respectively. We studied the effect of isomerism in the diazinodiazine backbone on the HOFs of the designed compounds. In diazine isomers, pyridazine (278.5 kJ/mol) exhibits higher HOF than pyrimidine (185.4 kJ/mol) and pyrazine (203.9 kJ/mol). Hence, it is evident that the presence of pyridazine in fused rings will help to gain better HOF over pyrimidine and pyrazine. The fusion of pyrimidine-pyrazine (B3), pyrazine-pyrazine (B4), and pyrimidine-pyrimidine (B8, B9) rings shows HOF between 352 and 379 kJ/mol, while pyridazine-pyrazine (B1, B2), pyridazine-pyrimidine (B5–7), and pyridazine-pyridazine (B10–13) backbone show HOF between 449 and 558 kJ/mol (see Fig. 1). The  $HOF_{Gas}$  of tetranitro-diazinodiazines was computed by using the isodesmic reaction method (see Figure S15). With the incorporation of four  $-NO_2$  groups in the diazinodiazine backbone, their  $HOF_{Gas}$  increases by 50–105 kJ/mol, indicating that  $-NO_2$  group improves the energy content. It is noteworthy that all the diazinodiazine isomers possess four  $-NO_2$  groups, and hence, their HOF values depend on energy contribution from the backbone and position of  $-NO_2$  groups on the ring. The four diazinodiazine isomers (P10–13) with fused pyridazine rings exhibit high  $HOF_{Solid}$  among the designed compounds. The highest  $HOF_{Solid}$  is for P10 (556 kJ/mol), which has the fused pyridazine rings, and four  $-NO_2$  groups kept close to each other on the backbone. Overall, all the tetranitro-diazinodiazines show endothermic  $HOF_{Solid}$  ranging from 296 (P9) to 556 (P10) kJ/mol caused by the high energy contribution from the diazinodiazine backbone (see Fig. 1) and  $-NO_2$  groups.

**Table 1** Computed total energies ( $E_0$ ), zero-point energies (ZPE), thermal correction ( $H_T$ ), and gas-phase HOF ( $HOF_{Gas}$ ) of the diazinodiazine isomers

Compd.	$E_0$ (a.u.)	ZPE (a.u.)	$H_T$ (a.u.)	$HOF_{Gas}$ (kJ/mol)	
				G4 method	Isodesmic reaction method
B1	–449.720565	0.0996	0.0073	466.7	470.3
B2	–449.722106	0.0997	0.0073	461.5	466.3
B3	–449.758357	0.1005	0.0073	366.4	380.4
B4	–449.754088	0.1003	0.0072	379.3	374.7
B5	–449.723299	0.0997	0.0074	457.8	480.0
B6	–449.726172	0.0999	0.0074	449.3	472.5
B7	–449.726903	0.0999	0.0074	449.7	470.6
B8	–449.763014	0.1008	0.0073	352.5	385.1
B9	–449.761783	0.1007	0.0073	356.4	388.3
B10	–449.685415	0.0988	0.0074	558.2	570.1
B11	–449.689517	0.0990	0.0074	547.0	559.4
B12	–449.689713	0.0990	0.0074	549.1	558.8
B13	–449.689772	0.0990	0.0075	544.8	558.7

**Table 2** Computed total energies ( $E_0$ ), zero-point energies (ZPE), thermal correction ( $H_T$ ), and HOFs for the tetranitro-diazinodiazines

Compd.	$E_0$ (a.u.)	ZPE (a.u.)	$H_T$ (a.u.)	HOF <sub>Gas</sub> (kJ/mol)	HOF <sub>Sub</sub> (kJ/mol)	HOF <sub>Solid</sub> (kJ/mol)
P1	-1267.308648	0.1077	0.0183	544.1	114.7	429.4
P2	-1267.310213	0.1076	0.0185	538.8	115.3	423.5
P3	-1267.354196	0.1085	0.0184	423.4	117.9	305.5
P4	-1267.351147	0.1085	0.0181	433.0	113.6	319.4
P5	-1267.309467	0.1078	0.0182	540.2	111.7	428.5
P6	-1267.314250	0.1078	0.0184	526.6	111.9	414.8
P7	-1267.313127	0.1076	0.0186	532.0	116.0	416.1
P8	-1267.357959	0.1087	0.0183	411.8	113.6	298.2
P9	-1267.356616	0.1084	0.0186	416.0	120.1	295.9
P10	-1267.262818	0.1070	0.0182	663.5	107.5	556.1
P11	-1267.268287	0.1069	0.0185	648.8	108.7	540.2
P12	-1267.267779	0.1068	0.0184	652.7	112.7	540.0
P13	-1267.270338	0.1072	0.0181	641.9	104.8	537.1

## Detonation performance

Oxygen balance (OB) and density are the crucial properties contributing to the detonation performance of an energetic molecule. All of the tetranitro-diazinodiazines possess a negative OB (−20.5 %), indicating the oxygen deficiency in a molecule that is necessary to transform all hydrogen into  $H_2O$  and all carbon into  $CO_2$ . The OB values of tetranitro-diazinodiazines are comparable to RDX and HMX (−21.6%). The densities of tetranitro-diazinodiazines were predicted by using the Politzer method [26] based on electrostatic interaction index and molecular surface properties (see Table S2). The predicted densities of the tetranitro-diazinodiazines range from 1.87–1.89  $g/cm^3$ , which are more significant than RDX (1.80  $g/cm^3$ ) and close to HMX (1.90  $g/cm^3$ ) [27]. The higher densities of these compounds may be owed to the coplanar

fused heterocyclic backbone and four  $-NO_2$  groups. The detonation properties were predicted by the Kamlet-Jacobs equation [28]. The computed detonation velocities and pressures of the tetranitro-diazinodiazines are in the range from 8.36 (P9) to 8.68 (P13) km/s and from 31.72 (P9) to 34.42 (P13) GPa, respectively (see Table 3). The higher detonation properties originate from the high energy content, density, and OB, benefited from the nitrogen-rich fused backbone and  $-NO_2$  groups. The fusion of pyrimidine and pyrazine rings (P3, P4, P8, and P9) reveals slightly lower detonation performance than the pyridazine ring in the fused backbone. P10–13 displays the best performance, having calculated detonation velocities exceeding 8.65 km/s and detonation pressures above 34.09 GPa, mainly due to their high HOF<sub>Solid</sub>. These values are comparable to those of RDX (8.60 km/s, 33.92 GPa) [27]. All the tetranitro-diazinodiazines show detonation properties

**Table 3** Predicted densities and detonation properties the tetranitro-diazinodiazines

Compd.	Density ( $g/cm^3$ )	Detonation velocity (km/s)	Detonation pressure (GPa)	$Q$ (cal/g)
P1	1.88	8.54	33.18	1534
P2	1.87	8.50	32.78	1530
P3	1.88	8.40	32.14	1439
P4	1.87	8.39	31.92	1450
P5	1.89	8.57	33.53	1533
P6	1.88	8.52	33.06	1523
P7	1.87	8.49	32.72	1524
P8	1.88	8.40	32.08	1434
P9	1.87	8.36	31.72	1432
P10	1.88	8.67	34.21	1631
P11	1.88	8.65	34.09	1619
P12	1.88	8.65	34.09	1619
P13	1.89	8.68	34.42	1617

**Table 4** Computed parameters to evaluate and interpret the sensitivity of tetranitro-diazinodiazines

Compd.	C–NO <sub>2</sub> (Å)	BDE (kJ/mol)	–Q <sub>NO<sub>2</sub></sub> (e)	V <sub>eff</sub> (Å <sup>3</sup> )	V <sub>int</sub> (Å <sup>3</sup> )	ΔV (Å <sup>3</sup> )
P1	1.4849	209.58	0.277	275.6	206.8	69
P2	1.4836	209.41	0.250	277.5	207.2	70
P3	1.4939	232.94	0.264	276.3	206.8	70
P4	1.4839	210.38	0.258	276.7	206.6	70
P5	1.4940	232.12	0.295	274.7	206.7	68
P6	1.4935	230.76	0.263	276.4	206.8	70
P7	1.4929	231.48	0.268	277.0	207.1	70
P8	1.4928	230.18	0.258	275.5	206.5	69
P9	1.4945	233.47	0.266	277.0	206.9	70
P10	1.4787	222.34	0.301	275.2	207.0	68
P11	1.4840	209.77	0.289	276.4	207.2	69
P12	1.4847	229.98	0.277	275.6	206.9	69
P13	1.4835	207.55	0.253	274.7	206.6	68

better than TNT (6.94 km/s, 22 GPa) and TATB (8.11 km/s, 31.1 GPa) [27]. According to earlier report [28], 4N<sub>2</sub>(g), 4CO<sub>2</sub>(g), and 2C(s) are expected to be the detonation products of P1–P13 (C<sub>6</sub>N<sub>8</sub>O<sub>8</sub>).

### Sensitivity correlation

A suitable balance between superior detonation performance and lower sensitivity for practical application and safety is crucial in designing new energetic materials. In this work, bond dissociation energies (BDE), detonation heat release per gram (Q), free space in the crystal lattice (ΔV), and charge on –NO<sub>2</sub> group (Q<sub>NO<sub>2</sub></sub>) are used for sensitivity comparison with RDX and HMX (see Tables 3 and 4) [29–31]. BDE indicates the stability of a chemical bond, where the higher value of BDE specifies the stronger bond and difficulty to rupture. Generally, a BDE more than 120 kJ/mol reveals the stability chemical bond [32, 33]. The bond lengths of the longest C–NO<sub>2</sub> range from 1.4835 to 1.4945 Å. All of the tetranitro-diazinodiazines have BDEs above 200 kJ/mol and are expected to exhibit good stability owing to their aromatic fused backbone. The computed BDEs for the longest N–NO<sub>2</sub> bond in RDX and HMX are 141 and 152 kJ/mol, respectively. Politzer and Murray [34] demonstrated that from the perspective of sensitivity, large Q values are not preferable. Higher Q values indicate greater sensitivity. The predicted Q values for tetranitro-diazinodiazines range from 1432 (P9) to 1631 (P10) cal/g (see Table 3). Computed Q values of compounds P1, P2, P5–7, and P10–13 are higher than RDX and HMX (1500 cal/g), and likely to be more sensitive. Politzer et al. [35–37] showed a correlation between free space (ΔV) available crystal lattice of energetic compound and impact sensitivity, where the greater ΔV value indicates more sensitivity of the compound. The ΔV values of tetranitro-diazinodiazines fall in the range of 68–70 Å<sup>3</sup> (see Table 4). This would make tetranitro-

diazinodiazines more sensitive than RDX (46 Å<sup>3</sup>) and HMX (49 Å<sup>3</sup>). Zhang et al. [38–40] suggested the correlation between net –NO<sub>2</sub> group charge and molecular stability. The more negative –NO<sub>2</sub> charge (–Q<sub>NO<sub>2</sub></sub>) stands for the more stable nitro compounds. The computed –Q<sub>NO<sub>2</sub></sub> charges of tetranitro-diazinodiazines range between 0.250 (P2) and 0.301 (P10) e, which are higher than RDX (0.105 e) and HMX (0.112 e), can be regarded as stable. The sensitivity predictions with BDE and Q<sub>NO<sub>2</sub></sub> approach show contradictory results to Q and ΔV method and do not correlate well. These results can be viewed as general trends and provide a crude evaluation of sensitivity for tetranitro-diazinodiazines. Application of uniform and specific approach/equation to estimate the sensitivity of newly designed compounds is very challenging as sensitivity is governed by many molecular, physical, and environmental factors and prone to significant uncertainties.

### Conclusions

Diazinodiazine and its tetranitro derivatives are theoretically studied at B3PW91/6-31G(d,p) level. The results exemplify the importance of planar, aromatic, and nitrogen-rich diazinodiazine fused backbone as valuable scaffolds for building potential, stable, and less sensitive energetic materials. The addition of nitro groups to the diazinodiazine backbone subsequently improves their energetic performance and leads to a combination of features that enhance HOF, oxygen balance, density, and performance. The HOFs relate to pyridazine, pyrimidine, and pyrazine rings in the fused backbone and the position of nitro groups. In terms of HOF, fused pyridazine rings have a significant advantage over both pyrimidine and pyrazine rings. The tetranitro-diazinodiazines show HOF > 295 kJ/mol, OB ≈ –20.5 %, density > 1.87



$\text{g/cm}^3$ ,  $D > 8.36 \text{ km/s}$ , and  $P > 31.72 \text{ GPa}$ . Our observations indicate that a combination of diazinodiazine isomers with suitable explosophoric groups could obtain potential energetic compounds while preserving molecular stability.

**Supplementary Information** The online version contains supplementary material available at <https://doi.org/10.1007/s11224-021-01791-1>.

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**Author contribution** Anjali Maan: conception and design, performed the computations and the numerical calculations, and acquisition of data.

Vikas Dasharath Ghule: designed the model and the computational framework, analysis and interpretation of data, drafting the article, and critical revision of the article

Srinivas Dharavath: analysis and interpretation of data and drafting the article

**Data availability** The authors confirm that the data supporting the findings of this study are available within the article and its [supplementary material](#).

**Code availability** All computations were performed with Gaussian 09 program and Multiwfn program. Gaussian 09 program can be obtained under academic or commercial license from Gaussian, Inc. (<https://gaussian.com/>). Multiwfn is available free of charge and open-source for both academic and commercial usages (<http://sobereva.com/multiwfn/>).

## Declarations

**Competing interests** The authors declare no competing interests.

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