# Supporting Information

# *Theoretical Studies of Pentazole based Compounds with High Detonation Performance*

Weijing Zhang a,Tonglai zhang a\*, Wei Guo b, Lin Wang a, Zhimin Li a and Jianguo Zhang a

1. State Key Laboratory of Explosion Science and Technology, School of Mechatronical Engineering, Beijing Institute of Technology, 5 South Zhongguancun Street, Beijing 100081, P. R. China.
2. School of Physics, Beijing Institute of Technology, 5 South Zhongguancun Street, Beijing 100081, P. R. China.

† E-mail: ztlbit@bit.edu.cn

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## Geometry in gas phase

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**Figure S1** Optimized geometry of **TATPB**

**Table S1** Bond length of **TATPB** in gas phase

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom1 | Atom2 | Length/Å | Atom1 | Atom2 | Length/Å |
| C1 | C2 | 1.4182 | N9 | N20 | 1.3366 |
| C1 | C6 | 1.4181 | N10 | H27 | 1.0079 |
| C1 | N12 | 1.4289 | N10 | H28 | 1.008 |
| C2 | C3 | 1.4192 | N11 | H29 | 1.0098 |
| C2 | N11 | 1.4369 | N11 | H30 | 1.0092 |
| C3 | C4 | 1.4217 | N12 | N21 | 1.3359 |
| C3 | N8 | 1.4276 | N12 | N24 | 1.3359 |
| C4 | C5 | 1.4216 | N13 | N14 | 1.2976 |
| C4 | N10 | 1.4308 | N14 | N15 | 1.3351 |
| C5 | C6 | 1.4192 | N15 | N16 | 1.2983 |
| C5 | N9 | 1.4277 | N17 | N18 | 1.2983 |
| C6 | N7 | 1.4369 | N18 | N19 | 1.3351 |
| N7 | H25 | 1.0093 | N19 | N20 | 1.2975 |
| N7 | H26 | 1.0096 | N21 | N22 | 1.2967 |
| N8 | N13 | 1.3367 | N22 | N23 | 1.3379 |
| N8 | N16 | 1.3357 | N23 | N24 | 1.2968 |
| N9 | N17 | 1.3357 |  |  |  |

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**Figure S2** Optimized geometry of **TATPH**

**Table S2** Bond length of **TATPH** in gas phase

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom1 | Atom2 | Length | Atom1 | Atom2 | Length |
| C1 | C2 | 1.5449 | N8 | N13 | 1.3256 |
| C1 | C6 | 1.5387 | N8 | N16 | 1.327 |
| C1 | N12 | 1.4719 | N9 | N17 | 1.3256 |
| C1 | H25 | 1.0921 | N9 | N20 | 1.3269 |
| C2 | C3 | 1.5388 | N10 | H33 | 1.0138 |
| C2 | N11 | 1.4594 | N10 | H34 | 1.0136 |
| C2 | H26 | 1.0979 | N11 | H35 | 1.0139 |
| C3 | C4 | 1.5448 | N11 | H36 | 1.0136 |
| C3 | N8 | 1.472 | N12 | N21 | 1.3256 |
| C3 | H27 | 1.0922 | N12 | N24 | 1.327 |
| C4 | C5 | 1.5388 | N13 | N14 | 1.2966 |
| C4 | N10 | 1.4593 | N14 | N15 | 1.3466 |
| C4 | H28 | 1.0978 | N15 | N16 | 1.2961 |
| C5 | C6 | 1.5449 | N17 | N18 | 1.2967 |
| C5 | N9 | 1.4719 | N18 | N19 | 1.3466 |
| C5 | H29 | 1.0921 | N19 | N20 | 1.2961 |
| C6 | N7 | 1.4593 | N21 | N22 | 1.2967 |
| C6 | H30 | 1.0979 | N22 | N23 | 1.3466 |
| N7 | H31 | 1.0139 | N23 | N24 | 1.2962 |
| N7 | H32 | 1.0136 |  |  |  |



**Figure S3** Optimized geometry of **TNTPB**

**Table S3** Bond length of **TNTPB** in gas phase

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom1 | Atom2 | Length | Atom1 | Atom2 | Length |
| C1 | C2 | 1.3943 | N9 | N21 | 1.3396 |
| C1 | C6 | 1.3944 | N10 | N11 | 1.2819 |
| C1 | N9 | 1.4121 | N11 | N12 | 1.3635 |
| C2 | C3 | 1.3943 | N12 | N13 | 1.2818 |
| C2 | N28 | 1.4929 | N14 | N15 | 1.2818 |
| C3 | C4 | 1.3944 | N15 | N16 | 1.3636 |
| C3 | N7 | 1.4121 | N16 | N17 | 1.2819 |
| C4 | C5 | 1.3945 | N18 | N19 | 1.2819 |
| C4 | N25 | 1.493 | N19 | N20 | 1.3634 |
| C5 | C6 | 1.3944 | N20 | N21 | 1.2818 |
| C5 | N8 | 1.4121 | N22 | O23 | 1.2128 |
| C6 | N22 | 1.4929 | N22 | O24 | 1.2128 |
| N7 | N10 | 1.3396 | N25 | O26 | 1.2128 |
| N7 | N13 | 1.3396 | N25 | O27 | 1.2128 |
| N8 | N14 | 1.3396 | N28 | O29 | 1.2127 |
| N8 | N17 | 1.3397 | N28 | O30 | 1.2128 |
| N9 | N18 | 1.3396 |  |  |  |

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**Figure S4** Optimized geometry of **TNTPH**

**Table S4** Bond length of **TNTPH** in gas phase

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom1 | Atom2 | Length | Atom1 | Atom2 | Length |
| C1 | C2 | 1.5357 | N8 | N14 | 1.332 |
| C1 | C6 | 1.5357 | N8 | N17 | 1.3335 |
| C1 | N9 | 1.4589 | N9 | N18 | 1.3321 |
| C1 | H31 | 1.0919 | N9 | N21 | 1.3334 |
| C2 | C3 | 1.5357 | N10 | N11 | 1.2885 |
| C2 | N28 | 1.5369 | N11 | N12 | 1.358 |
| C2 | H32 | 1.0892 | N12 | N13 | 1.2882 |
| C3 | C4 | 1.5357 | N14 | N15 | 1.2885 |
| C3 | N7 | 1.4589 | N15 | N16 | 1.3581 |
| C3 | H33 | 1.0918 | N16 | N17 | 1.2882 |
| C4 | C5 | 1.5359 | N18 | N19 | 1.2886 |
| C4 | N25 | 1.5369 | N19 | N20 | 1.3582 |
| C4 | H34 | 1.0891 | N20 | N21 | 1.2883 |
| C5 | C6 | 1.5356 | N22 | O23 | 1.2119 |
| C5 | N8 | 1.4589 | N22 | O24 | 1.2191 |
| C5 | H35 | 1.0919 | N25 | O26 | 1.2119 |
| C6 | N22 | 1.5368 | N25 | O27 | 1.2191 |
| C6 | H36 | 1.0891 | N28 | O29 | 1.2119 |
| N7 | N10 | 1.332 | N28 | O30 | 1.2191 |
| N7 | N13 | 1.3335 |  |  |  |

## Wiberg bond order index

**Table S5** Bond Order Index of **TATPB**

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Bond Order | Bond | Bond Order |
| C1-C2 | 1.2617 | C1-N12 | 0.9805 |
| C2-C3 | 1.2605 | C2-N11 | 1.2517 |
| C3-C4 | 1.2547 | C3-N8 | 0.9894 |
| C4-C5 | 1.2549 | C4-N10 | 1.2662 |
| C5-C6 | 1.2604 | C5-N9 | 0.9892 |
| C6-C1 | 1.2617 | C6-N7 | 1.2517 |
| N8-N13 | 1.2479 | N9-N17 | 1.2502 |
| N13-N14 | 1.5162 | N17-N18 | 1.5125 |
| N14-N15 | 1.3937 | N18-N19 | 1.3935 |
| N15-N16 | 1.5123 | N19-N20 | 1.5164 |
| N16-N8 | 1.2502 | N20-N9 | 1.2479 |
| N12-N21 | 1.2502 | N7-H25 | 0.7940 |
| N21-N22 | 1.5234 | N7-H26 | 0.7888 |
| N22-N23 | 1.3857 | N10-H27 | 0.7851 |
| N23-N24 | 1.5234 | N10-H28 | 0.7849 |
| N24-N12 | 1.2501 | N11-H29 | 0.7887 |
| N11-H30 | 0.7939 |  |  |

**Table S6** Bond Order Index of **TATPH**

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Bond Order | Bond | Bond Order |
| C1-C2 | 0.9677 | C1-N12 | 0.9162 |
| C2-C3 | 0.9719 | C2-N11 | 1.0134 |
| C3-C4 | 0.9677 | C3-N8 | 0.9162 |
| C4-C5 | 0.9719 | C4-N10 | 1.0134 |
| C5-C6 | 0.9676 | C5-N9 | 0.9163 |
| C6-C1 | 0.9719 | C6-N7 | 1.0134 |
| N8-N13 | 1.2750 | N9-N17 | 1.2750 |
| N13-N14 | 1.5413 | N17-N18 | 1.5413 |
| N14-N15 | 1.3705 | N18-N19 | 1.3705 |
| N15-N16 | 1.5436 | N19-N20 | 1.5437 |
| N16-N8 | 1.2735 | N20-N9 | 1.2735 |
| N12-N21 | 1.2750 | N7-H31 | 0.8400 |
| N21-N22 | 1.5413 | N7-H32 | 0.8506 |
| N22-N23 | 1.3705 | N10-H33 | 0.8400 |
| N23-N24 | 1.5436 | N10-H34 | 0.8506 |
| N24-N12 | 1.2736 | N11-H35 | 0.8400 |
| C1-H25 | 0.8878 | N11-H36 | 0.8506 |
| C2-H26 | 0.8939 | C3-H27 | 0.8878 |
| C4-H28 | 0.8939 | C5-H29 | 0.8878 |
| C6-H30 | 0.8939 |  |  |

**Table S7** Bond Order Index of **TNTPB**

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Bond Order | Bond | Bond Order |
| C1-C2 | 1.3511 | C1-N9 | 0.9805 |
| C2-C3 | 1.3511 | C2-N28 | 1.2517 |
| C3-C4 | 1.3511 | C3-N7 | 0.9894 |
| C4-C5 | 1.3512 | C4-N25 | 1.2662 |
| C5-C6 | 1.3511 | C5-N8 | 0.9892 |
| C6-C1 | 1.3512 | C6-N22 | 1.2517 |
| N8-N14 | 1.2127 | N9-N18 | 1.2127 |
| N14-N15 | 1.6162 | N18-N19 | 1.6163 |
| N15-N16 | 1.3066 | N19-N20 | 1.3066 |
| N16-N17 | 1.6163 | N20-N21 | 1.6163 |
| N17-N8 | 1.2127 | N21-N9 | 1.2127 |
| N7-N10 | 1.2127 | N22-O23 | 1.5314 |
| N10-N11 | 1.6162 | N22-O24 | 1.5314 |
| N11-N12 | 1.3066 | N25-O26 | 1.5314 |
| N12-N13 | 1.6163 | N25-O27 | 1.5314 |
| N13-N7 | 1.2127 | N28-O29 | 1.5314 |
| N28-O30 | 1.5314 |  |  |

**Table S8** Bond Order Index of **TNTPH**

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Bond Order | Bond | Bond Order |
| C1-C2 | 0.9742 | C1-N9 | 0.9162 |
| C2-C3 | 0.9742 | C2-N28 | 1.0134 |
| C3-C4 | 0.9742 | C3-N7 | 0.9162 |
| C4-C5 | 0.9742 | C4-N25 | 1.0134 |
| C5-C6 | 0.9742 | C5-N8 | 0.9163 |
| C6-C1 | 0.9742 | C6-N22 | 1.0134 |
| N8-N14 | 1.2393 | N9-N18 | 1.2393 |
| N14-N15 | 1.5837 | N18-N19 | 1.5837 |
| N15-N16 | 1.3348 | N19-N20 | 1.3348 |
| N16-N17 | 1.5880 | N20-N21 | 1.5880 |
| N17-N8 | 1.2447 | N21-N9 | 1.2447 |
| N7-N10 | 1.2393 | N22-O23 | 1.5592 |
| N10-N11 | 1.5837 | N22-O24 | 1.5194 |
| N11-N12 | 1.3348 | N25-O26 | 1.5592 |
| N12-N13 | 1.5880 | N25-O27 | 1.5194 |
| N13-N7 | 1.2447 | N28-O29 | 1.5592 |
| C1-H31 | 0.8678 | N28-O30 | 1.5194 |
| C2-H32 | 0.8871 | C3-H33 | 0.8678 |
| C4-H34 | 0.8871 | C5-H35 | 0.8679 |
| C6-H36 | 0.8871 |  |  |

## Test for calculation parameters



**Figure S5** Test of KPOINTS for solid phase of **TNTPB** in *P*



**Figure S6** Test of KPOINTS for solid phase of **TNTPB** in *P*21/c



**Figure S6** Test of energy cutoff for solid phases of **TNTPB** in *P* and *P*21/c based on lattice energy

## Geometry in solid phase

**Table S9** Bond length of **TNTPB** in *P* space group

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom1 | Atom2 | Length | Atom1 | Atom2 | Length |
| C1 | C3 | 1.4006 | C2 | C4 | 1.4006 |
| C1 | C11 | 1.4005 | C2 | C12 | 1.4005 |
| C1 | N5 | 1.4071 | C2 | N6 | 1.4071 |
| C3 | C5 | 1.3984 | C4 | C6 | 1.3984 |
| C3 | N35 | 1.489 | C4 | N36 | 1.489 |
| C5 | C7 | 1.3991 | C6 | C8 | 1.3991 |
| C5 | N1 | 1.4137 | C6 | N2 | 1.4137 |
| C7 | C9 | 1.3992 | C8 | C10 | 1.3992 |
| C7 | N33 | 1.4926 | C8 | N34 | 1.4926 |
| C9 | C11 | 1.3989 | C10 | C12 | 1.3989 |
| C9 | N3 | 1.4136 | C10 | N4 | 1.4136 |
| C11 | N31 | 1.4896 | C12 | N32 | 1.4896 |
| N1 | N7 | 1.3466 | N2 | N8 | 1.3466 |
| N1 | N13 | 1.3433 | N2 | N14 | 1.3433 |
| N3 | N15 | 1.3432 | N4 | N16 | 1.3433 |
| N3 | N21 | 1.3465 | N4 | N22 | 1.3465 |
| N5 | N23 | 1.347 | N6 | N24 | 1.347 |
| N5 | N29 | 1.3476 | N6 | N30 | 1.3476 |
| N7 | N9 | 1.2941 | N8 | N10 | 1.2941 |
| N9 | N11 | 1.365 | N10 | N12 | 1.365 |
| N11 | N13 | 1.2959 | N12 | N14 | 1.2959 |
| N15 | N17 | 1.296 | N16 | N18 | 1.296 |
| N17 | N19 | 1.3649 | N18 | N20 | 1.3649 |
| N19 | N21 | 1.2941 | N20 | N22 | 1.2941 |
| N23 | N25 | 1.2926 | N24 | N26 | 1.2926 |
| N25 | N27 | 1.3681 | N26 | N28 | 1.3681 |
| N27 | N29 | 1.2925 | N28 | N30 | 1.2925 |
| N31 | O1 | 1.2336 | N32 | O2 | 1.2336 |
| N31 | O3 | 1.2287 | N32 | O4 | 1.2287 |
| N33 | O5 | 1.2282 | N34 | O6 | 1.2282 |
| N33 | O7 | 1.2281 | N34 | O8 | 1.2281 |
| N35 | O9 | 1.2285 | N36 | O10 | 1.2285 |
| N35 | O11 | 1.2337 | N36 | O12 | 1.2337 |

**Table S10** Bond length of **TNTPB** in *P*21/c space group

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atom1 | Atom2 | Length | Atom1 | Atom2 | Length |
| C1 | C5 | 1.398 | C3 | C7 | 1.398 |
| C1 | C21 | 1.4008 | C3 | C23 | 1.4008 |
| C1 | N9 | 1.4237 | C3 | N11 | 1.4237 |
| C5 | C9 | 1.4035 | C7 | C11 | 1.4035 |
| C5 | N69 | 1.4901 | C7 | N71 | 1.4901 |
| C9 | C13 | 1.4035 | C11 | C15 | 1.4035 |
| C9 | N1 | 1.4067 | C11 | N3 | 1.4067 |
| C13 | C17 | 1.3979 | C15 | C19 | 1.3979 |
| C13 | N65 | 1.4901 | C15 | N67 | 1.4901 |
| C17 | C21 | 1.4008 | C19 | C23 | 1.4008 |
| C17 | N5 | 1.4237 | C19 | N7 | 1.4237 |
| C21 | N61 | 1.4929 | C23 | N63 | 1.4928 |
| N1 | N13 | 1.3502 | N3 | N15 | 1.3502 |
| N1 | N25 | 1.3502 | N3 | N27 | 1.3502 |
| N5 | N29 | 1.3439 | N7 | N31 | 1.3439 |
| N5 | N41 | 1.3457 | N7 | N43 | 1.3458 |
| N9 | N45 | 1.3439 | N11 | N47 | 1.3439 |
| N9 | N57 | 1.3458 | N11 | N59 | 1.3458 |
| N13 | N17 | 1.2893 | N15 | N19 | 1.2893 |
| N17 | N21 | 1.3734 | N19 | N23 | 1.3734 |
| N21 | N25 | 1.2893 | N23 | N27 | 1.2893 |
| N29 | N33 | 1.2953 | N31 | N35 | 1.2953 |
| N33 | N37 | 1.3606 | N35 | N39 | 1.3606 |
| N37 | N41 | 1.296 | N39 | N43 | 1.296 |
| N45 | N49 | 1.2953 | N47 | N51 | 1.2953 |
| N49 | N53 | 1.3606 | N51 | N55 | 1.3606 |
| N53 | N57 | 1.296 | N55 | N59 | 1.296 |
| N61 | O1 | 1.2294 | N63 | O3 | 1.2294 |
| N61 | O5 | 1.2294 | N63 | O7 | 1.2294 |
| N65 | O9 | 1.2272 | N67 | O11 | 1.2272 |
| N65 | O13 | 1.2327 | N67 | O15 | 1.2327 |
| N69 | O17 | 1.2327 | N71 | O19 | 1.2327 |
| N69 | O21 | 1.2272 | N71 | O23 | 1.2272 |
| C2 | C6 | 1.3979 | C4 | C8 | 1.3979 |
| C2 | C22 | 1.4008 | C4 | C24 | 1.4008 |
| C2 | N10 | 1.4237 | C4 | N12 | 1.4237 |
| C6 | C10 | 1.4035 | C8 | C12 | 1.4035 |
| C6 | N70 | 1.4901 | C8 | N72 | 1.4901 |
| C10 | C14 | 1.4035 | C12 | C16 | 1.4035 |
| C10 | N2 | 1.4067 | C12 | N4 | 1.4067 |
| C14 | C18 | 1.3979 | C16 | C20 | 1.3979 |
| C14 | N66 | 1.4901 | C16 | N68 | 1.4901 |
| C18 | C22 | 1.4008 | C20 | C24 | 1.4008 |
| C18 | N6 | 1.4237 | C20 | N8 | 1.4237 |
| C22 | N62 | 1.4929 | C24 | N64 | 1.4929 |
| N2 | N14 | 1.3502 | N4 | N16 | 1.3502 |
| N2 | N26 | 1.3502 | N4 | N28 | 1.3502 |
| N6 | N30 | 1.3439 | N8 | N32 | 1.3439 |
| N6 | N42 | 1.3458 | N8 | N44 | 1.3458 |
| N10 | N46 | 1.3439 | N12 | N48 | 1.3439 |
| N10 | N58 | 1.3458 | N12 | N60 | 1.3458 |
| N14 | N18 | 1.2893 | N16 | N20 | 1.2893 |
| N18 | N22 | 1.3734 | N20 | N24 | 1.3734 |
| N22 | N26 | 1.2893 | N24 | N28 | 1.2893 |
| N30 | N34 | 1.2953 | N32 | N36 | 1.2953 |
| N34 | N38 | 1.3606 | N36 | N40 | 1.3606 |
| N38 | N42 | 1.296 | N40 | N44 | 1.296 |
| N46 | N50 | 1.2953 | N48 | N52 | 1.2953 |
| N50 | N54 | 1.3606 | N52 | N56 | 1.3606 |
| N54 | N58 | 1.296 | N56 | N60 | 1.296 |
| N62 | O2 | 1.2294 | N64 | O4 | 1.2294 |
| N62 | O6 | 1.2294 | N64 | O8 | 1.2294 |
| N66 | O10 | 1.2272 | N68 | O12 | 1.2272 |
| N66 | O14 | 1.2327 | N68 | O16 | 1.2327 |
| N70 | O18 | 1.2327 | N72 | O20 | 1.2327 |
| N70 | O22 | 1.2272 | N72 | O24 | 1.2272 |