

# Stability, electronic and optical properties of two-dimensional phosphoborane

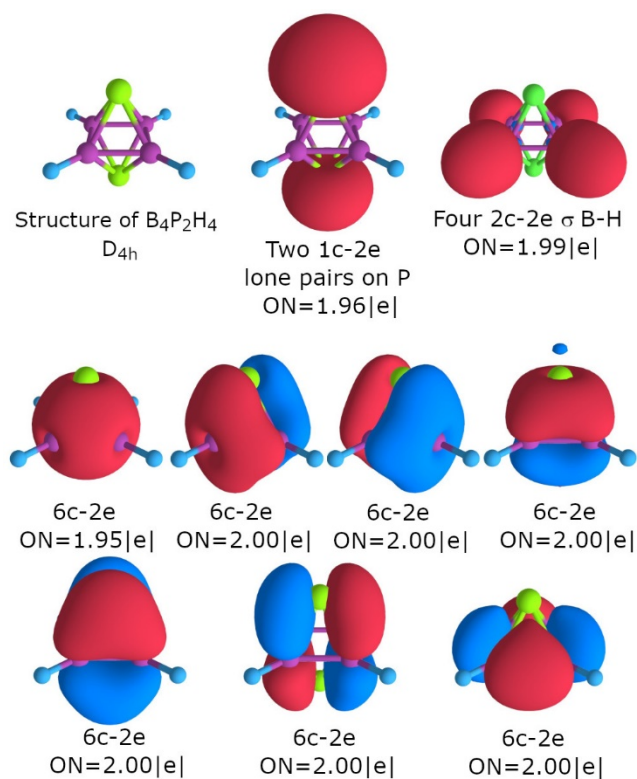
D.V. Steglenko, N.V. Tkachenko, A.I. Boldyrev, R.M. Minyaev, V.I. Minkin

## Supporting Information

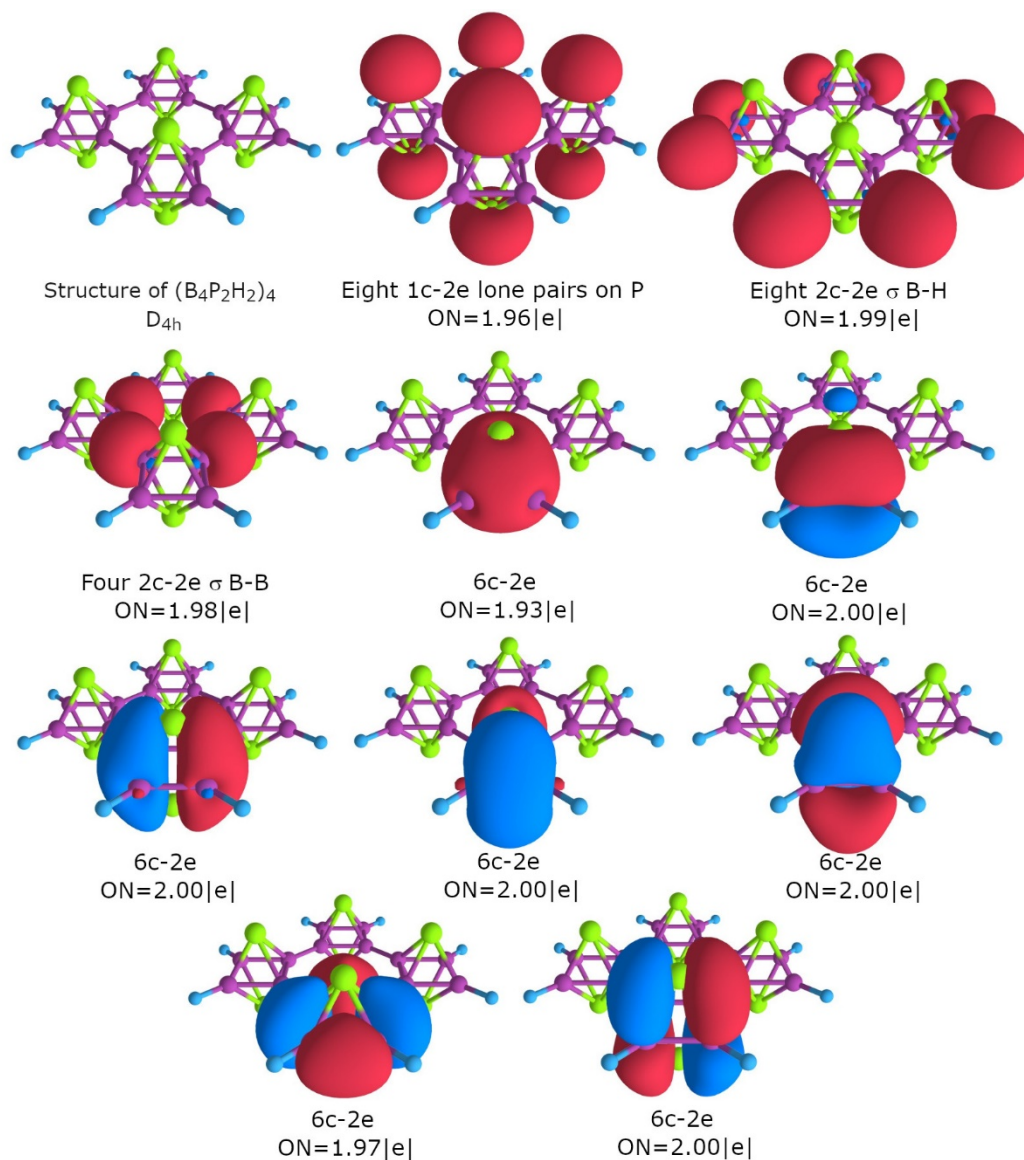
### Contents

|   |    |
|---|----|
| 1. Chemical bonding patterns of the $B_4P_2H_4$ and $(B_4P_2)_4H_8$ clusters.. .. | S2 |
| 2. Cartesian coordinates of the investigated clusters.....                        | S4 |

## 1. Chemical bonding patterns of the $B_4P_2H_4$ and $(B_4P_2)_4H_8$ clusters.



**Figure S1.** Chemical bonding pattern obtained for the  $B_4P_2H_4$  cluster. ON denotes the occupation number of a certain bond. Boron atoms are purple, phosphorous atoms are green, and hydrogen atoms are light blue.



**Figure S2.** Chemical bonding pattern obtained for the tetramer of phosphoborane. ON denotes the occupation number of a certain bond. Boron atoms are purple, phosphorous atoms are green, and hydrogen atoms are light blue.

## 2. Cartesian coordinates of the investigated clusters.

**Table S1.** Cartesian coordinates of the investigated clusters.

|   |   |              |              |              |
|---|---|--------------|--------------|--------------|
| $D_{4h}$ - $B_4P_2H_4$ (singlet spin state)     | PBE0/def2-TZVP<br>Total electronic energy: -784.228962071 H<br>0 imaginary frequencies  |              |              |              |
|   | 5   | 0.000000000  | 1.259264000  | 0.000000000  |
|   | 5   | -1.259264000 | 0.000000000  | 0.000000000  |
|   | 5   | 0.000000000  | -1.259264000 | 0.000000000  |
|   | 5   | 1.259264000  | 0.000000000  | 0.000000000  |
|   | 15  | 0.000000000  | 0.000000000  | -1.493380000 |
|   | 15  | 0.000000000  | 0.000000000  | 1.493380000  |
|   | 1   | 0.000000000  | -2.442491000 | 0.000000000  |
|   | 1   | 2.442491000  | 0.000000000  | 0.000000000  |
|   | 1   | -2.442491000 | 0.000000000  | 0.000000000  |
|   | 1   | 0.000000000  | 2.442491000  | 0.000000000  |
| $D_{4h}$ - $(B_4P_2H_2)_4$ (singlet spin state) | The optimized geometry of the 2D- $B_4P_2$ . Free valences at boron atoms were terminated by hydrogen atoms with a bond length B-H = 1.183 Å. |              |              |              |
|   | 5   | -0.832993000 | 2.115972000  | 0.000000000  |
|   | 5   | -0.832993000 | -2.115972000 | 0.000000000  |
|   | 5   | 2.115972000  | 3.398950000  | 0.000000000  |
|   | 5   | -2.115972000 | 3.398950000  | 0.000000000  |
|   | 5   | 2.115972000  | -0.832993000 | 0.000000000  |
|   | 5   | -2.115972000 | -0.832993000 | 0.000000000  |
|   | 5   | 0.832993000  | 2.115972000  | 0.000000000  |
|   | 5   | -3.398950000 | 2.115972000  | 0.000000000  |
|   | 5   | 0.832993000  | -2.115972000 | 0.000000000  |
|   | 5   | -3.398950000 | -2.115972000 | 0.000000000  |
|   | 5   | 2.115972000  | 0.832993000  | 0.000000000  |
|   | 5   | -2.115972000 | 0.832993000  | 0.000000000  |
|   | 5   | 2.115972000  | -3.398950000 | 0.000000000  |
|   | 5   | -2.115972000 | -3.398950000 | 0.000000000  |
|   | 15  | 2.115972000  | 2.115972000  | 1.489689000  |
|   | 15  | -2.115972000 | 2.115972000  | 1.489689000  |
|   | 15  | 2.115972000  | -2.115972000 | 1.489689000  |
|   | 15  | -2.115972000 | -2.115972000 | 1.489689000  |
|   | 15  | 2.115972000  | 2.115972000  | -1.489689000 |
|   | 15  | -2.115972000 | 2.115972000  | -1.489689000 |
|   | 15  | 2.115972000  | -2.115972000 | -1.489689000 |
|   | 15  | -2.115972000 | -2.115972000 | -1.489689000 |
|   | 5   | 3.398950000  | 2.115972000  | 0.000000000  |
|   | 5   | 3.398950000  | -2.115972000 | 0.000000000  |
|   | 1   | -2.115971000 | -4.582150000 | 0.000000000  |
|   | 1   | -4.582150000 | -2.115971000 | 0.000000000  |
|   | 1   | 2.115971000  | -4.582150000 | 0.000000000  |

|  |   |              |              |             |
|--|---|--------------|--------------|-------------|
|  | 1 | 4.582150000  | -2.115971000 | 0.000000000 |
|  | 1 | 4.582150000  | 2.115971000  | 0.000000000 |
|  | 1 | 2.115971000  | 4.582150000  | 0.000000000 |
|  | 1 | -2.115971000 | 4.582150000  | 0.000000000 |
|  | 1 | -4.582150000 | 2.115971000  | 0.000000000 |