|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| bond | AlPNT | AlPNT/CO2 | AlPNT/CS2 | AlPNT/H2S | AlPNT/H2Se | AlPNT/SO2 |
| Al1-P11 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 |
| Al1-P13 | 2.31 | 2.31 | 2.31 | 2.30 | 2.30 | 2.31 |
| Al2-P11 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 | 2.33 |
| Al2-P14 | 2.31 | 2.31 | 2.31 | 2.31 | 2.31 | 2.30 |
| Al2-P12 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 |
| Al3-P12 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 | 2.32 |
| Al3-P15 | 2.31 | 2.31 | 2.31 | 2.30 | 2.30 | 2.30 |
| Al4-P13 | 2.31 | 2.31 | 2.31 | 2.31 | 2.31 | 2.31 |
| Al4-P16 | 2.31 | 2.30 | 2.31 | 2.29 | 2.29 | 2.33 |
| Al4-P14 | 2.31 | 2.32 | 2.31 | 2.33 | 2.33 | 2.29 |
| Al5-P14 | 2.31 | 2.32 | 2.31 | 2.33 | 2.33 | 2.35 |
| Al5-P17 | 2.31 | 2.30 | 2.31 | 2.29 | 2.29 | 2.43 |
| Al5-P15 | 2.31 | 2.31 | 2.31 | 2.31 | 2.31 | 2.35 |
| Al6-P16 | 2.31 | 2.31 | 2.31 | 2.30 | 2.30 | 2.31 |
| Al6-P18 | 2.31 | 2.30 | 2.31 | 2.30 | 2.30 | 2.31 |
| Al7-P16 | 2.31 | 2.33 | 2.31 | 2.35 | 2.35 | 2.28 |
| Al7-P17 | 2.31 | 2.33 | 2.31 | 2.35 | 2.34 | 2.34 |
| Al7-P19 | 2.31 | 2.32 | 2.31 | 2.34 | 2.34 | 2.29 |
| Al8-P17 | 2.31 | 2.31 | 2.31 | 2.30 | 2.30 | 2.35 |
| Al8-P20 | 2.31 | 2.31 | 2.31 | 2.30 | 2.30 | 2.29 |
| Al9-P18 | 2.31 | 2.31 | 2.31 | 2.31 | 2.31 | 2.30 |
| Al9-P19 | 2.31 | 2.30 | 2.31 | 2.31 | 2.30 | 2.32 |
| Al10-P19 | 2.31 | 2.30 | 2.30 | 2.30 | 2.29 | 2.31 |
| Al10-P20 | 2.31 | 2.30 | 2.30 | 2.31 | 2.31 | 2.31 |

**Table S1.** The bond length (in Å) in pristine AlPNT and different studied models.

**Table S2.** The topological properties of electron density, total electron energy densities and its components at the critical point (in a.u.).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | CO2 | | | | |  | CS2 | | | | |  | H2S | | | |  |
| bond length | ρ | ρ | G | V | H | **bond length** | ρ | ρ | G | V | H | **bond length** | ρ | ρ | G | V | H |
| Al1-P11 | 0.0638 | 0.1170 | 0.0488 | -0.0683 | -0.0195 | **Al1-P11** | 0.0640 | 0.1175 | 0.0490 | -0.0686 | -0.0196 | **Al1-P11** | 0.0637 | 0.1168 | 0.0486 | -0.0681 | -0.0194 |
| Al1-P13 | 0.0641 | 0.1253 | 0.0503 | -0.0693 | -0.0190 | **Al1-P13** | 0.0640 | 0.1246 | 0.0501 | -0.0691 | -0.0190 | **Al1-P13** | 0.0643 | 0.1273 | 0.0509 | -0.0699 | -0.0190 |
| Al2-P11 | 0.0640 | 0.1174 | 0.0490 | -0.0687 | -0.0196 | **Al2-P11** | 0.0640 | 0.1174 | 0.0489 | -0.0685 | -0.0196 | **Al2-P11** | 0.0640 | 0.1171 | 0.0489 | -0.0686 | -0.0197 |
| Al2-P14 | 0.0637 | 0.1241 | 0.0499 | -0.0687 | -0.0189 | **Al2-P14** | 0.0640 | 0.1245 | 0.0501 | -0.0691 | -0.0190 | **Al2-P14** | 0.0635 | 0.1220 | 0.0494 | -0.0682 | -0.0189 |
| Al2-P12 | 0.0640 | 0.1175 | 0.0490 | -0.0687 | -0.0196 | **Al2-P12** | 0.0640 | 0.1176 | 0.0490 | -0.0686 | -0.0196 | **Al2-P12** | 0.0640 | 0.1171 | 0.0489 | -0.0686 | -0.0197 |
| Al3-P12 | 0.0639 | 0.1170 | 0.0488 | -0.0683 | -0.0195 | **Al3-P12** | 0.0640 | 0.1174 | 0.0490 | -0.0685 | -0.0196 | **Al3-P12** | 0.0637 | 0.1168 | 0.0487 | -0.0681 | -0.0194 |
| Al3-P15 | 0.0641 | 0.1252 | 0.0503 | -0.0693 | -0.0190 | **Al3-P15** | 0.0640 | 0.1248 | 0.0502 | -0.0692 | -0.0190 | **Al3-P15** | 0.0643 | 0.1271 | 0.0508 | -0.0698 | -0.0190 |
| Al4-P13 | 0.0626 | 0.1198 | 0.0483 | -0.0667 | -0.0184 | **Al4-P13** | 0.0626 | 0.1194 | 0.0482 | -0.0666 | -0.0184 | **Al4-P13** | 0.0626 | 0.1209 | 0.0485 | -0.0668 | -0.0183 |
| Al4-P16 | 0.0647 | 0.1285 | 0.0514 | -0.0706 | -0.0193 | **Al4-P16** | 0.0642 | 0.1248 | 0.0503 | -0.0695 | -0.0191 | **Al4-P16** | 0.0656 | 0.1338 | 0.0529 | -0.0724 | -0.0195 |
| Al4-P14 | 0.0622 | 0.1185 | 0.0478 | -0.0660 | -0.0182 | **Al4-P14** | 0.0626 | 0.1195 | 0.0483 | -0.0667 | -0.0184 | **Al4-P14** | 0.0614 | 0.1141 | 0.0464 | -0.0643 | -0.0179 |
| Al5-P14 | 0.0622 | 0.1184 | 0.0478 | -0.0659 | -0.0182 | **Al5-P14** | 0.0627 | 0.1197 | 0.0483 | -0.0667 | -0.0184 | **Al5-P14** | 0.0614 | 0.1141 | 0.0465 | -0.0644 | -0.0179 |
| Al5-P17 | 0.0647 | 0.1281 | 0.0513 | -0.0706 | -0.0193 | **Al5-P17** | 0.0642 | 0.1247 | 0.0503 | -0.0694 | -0.0191 | **Al5-P17** | 0.0654 | 0.1324 | 0.0526 | -0.0721 | -0.0195 |
| Al5-P15 | 0.0626 | 0.1200 | 0.0484 | -0.0667 | -0.0184 | **Al5-P15** | 0.0626 | 0.1196 | 0.0483 | -0.0666 | -0.0184 | **Al5-P15** | 0.0626 | 0.1207 | 0.0484 | -0.0667 | -0.0182 |
| Al6-P16 | 0.0633 | 0.1249 | 0.0497 | -0.0681 | -0.0184 | **Al6-P16** | 0.0630 | 0.1218 | 0.0489 | -0.0674 | -0.0185 | **Al6-P16** | 0.0639 | 0.1301 | 0.0510 | -0.0694 | -0.0184 |
| Al6-P18 | 0.0643 | 0.1270 | 0.0508 | -0.0698 | -0.0190 | **Al6-P18** | 0.0641 | 0.1258 | 0.0505 | -0.0695 | -0.0190 | **Al6-P18** | 0.0643 | 0.1281 | 0.0510 | -0.0699 | -0.0190 |
| Al7-P16 | 0.0620 | 0.1135 | 0.0468 | -0.0653 | -0.0185 | **Al7-P16** | 0.0629 | 0.1209 | 0.0487 | -0.0671 | -0.0185 | **Al7-P16** | 0.0598 | 0.1095 | 0.0445 | -0.0617 | -0.0172 |
| Al7-P17 | 0.0620 | 0.1135 | 0.0468 | -0.0653 | -0.0184 | **Al7-P17** | 0.0629 | 0.1210 | 0.0487 | -0.0672 | -0.0185 | **Al7-P17** | 0.0595 | 0.1085 | 0.0441 | -0.0612 | -0.0170 |
| Al7-P19 | 0.0638 | 0.1189 | 0.0490 | -0.0684 | -0.0193 | **Al7-P19** | 0.0640 | 0.1248 | 0.0502 | -0.0693 | -0.0190 | **Al7-P19** | 0.0616 | 0.1136 | 0.0466 | -0.0647 | -0.0182 |
| Al8-P17 | 0.0633 | 0.1248 | 0.0497 | -0.0682 | -0.0185 | **Al8-P17** | 0.0630 | 0.1219 | 0.0489 | -0.0674 | -0.0185 | **Al8-P17** | 0.0638 | 0.1288 | 0.0507 | -0.0693 | -0.0185 |
| Al8-P20 | 0.0642 | 0.1269 | 0.0507 | -0.0696 | -0.0190 | **Al8-P20** | 0.0641 | 0.1261 | 0.0505 | -0.0695 | -0.0190 | **Al8-P20** | 0.0642 | 0.1280 | 0.0509 | -0.0697 | -0.0189 |
| Al9-P18 | 0.0629 | 0.1276 | 0.0498 | -0.0677 | -0.0179 | **Al9-P18** | 0.0631 | 0.1278 | 0.0500 | -0.0680 | -0.0180 | **Al9-P18** | 0.0626 | 0.1267 | 0.0495 | -0.0673 | -0.0178 |
| Al9-P19 | 0.0632 | 0.1275 | 0.0500 | -0.0682 | -0.0181 | **Al9-P19** | 0.0630 | 0.1277 | 0.0499 | -0.0679 | -0.0180 | **Al9-P19** | 0.0630 | 0.1268 | 0.0498 | -0.0679 | -0.0181 |
| Al10-P19 | 0.0633 | 0.1296 | 0.0505 | -0.0685 | -0.0181 | **Al10-P19** | 0.0631 | 0.1288 | 0.0502 | -0.0682 | -0.0180 | **Al10-P19** | 0.0633 | 0.1299 | 0.0505 | -0.0686 | -0.0181 |
| Al10-P20 | 0.0630 | 0.1289 | 0.0501 | -0.0681 | -0.0179 | **Al10-P20** | 0.0632 | 0.1289 | 0.0502 | -0.0683 | -0.0180 | **Al10-P20** | 0.0629 | 0.1289 | 0.0500 | -0.0678 | -0.0178 |
| Al7-O62 | 0.0138 | 0.0288 | 0.0071 | -0.0070 | 0.0001 | **P19-S62** | 0.0032 | 0.0075 | 0.0014 | -0.0010 | 0.0004 | **P14-H62** | 0.0050 | 0.0129 | 0.0026 | -0.0019 | 0.0007 |
| P14-O63 | 0.0024 | 0.0076 | 0.0014 | -0.0009 | 0.0005 | **P14-S63** | 0.0006 | 0.0015 | 0.0003 | -0.0001 | 0.0001 | **S61-Al7** | 0.0302 | 0.0610 | 0.0186 | -0.0219 | -0.0033 |
| C61-O62 | 0.4358 | 0.3784 | 0.7822 | -1.4698 | -0.6876 | **C61-S62** | 0.2407 | 0.4211 | 0.3376 | -0.5699 | -0.2323 | **H61-S62** | 0.2041 | -0.4941 | 0.1208 | -0.3652 | -0.2444 |
| C63-O62 | 0.4486 | 0.5891 | 0.8530 | -1.5588 | -0.7058 | **C61-S63** | 0.2417 | 0.4355 | 0.3419 | -0.5749 | -0.2330 | **H63-S62** | 0.2052 | -0.5000 | 0.1216 | -0.3683 | -0.2467 |

**Continue of Table S2.** The topological properties of electron density, total electron energy densities and its components at the critical point (in a.u.).

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | H2Se | | | |  |  | SO2 | | | |  |
| bond length | ρ | 2ρ | G | V | H | **bond length** | ρ | 2ρ | G | V | H |
| Al1-P11 | 0.0637 | 0.1170 | 0.0487 | -0.0682 | -0.0194 | **Al1-P11** | 0.0646 | 0.1192 | 0.0497 | -0.0697 | -0.0199 |
| Al1-P13 | 0.0643 | 0.1276 | 0.0509 | -0.0700 | -0.0190 | **Al1-P13** | 0.0637 | 0.1249 | 0.0500 | -0.0687 | -0.0187 |
| Al2-P11 | 0.0640 | 0.1168 | 0.0488 | -0.0685 | -0.0196 | **Al2-P11** | 0.0632 | 0.1157 | 0.0481 | -0.0673 | -0.0192 |
| Al2-P14 | 0.0636 | 0.1218 | 0.0494 | -0.0684 | -0.0190 | **Al2-P14** | 0.0646 | 0.1284 | 0.0513 | -0.0705 | -0.0192 |
| Al2-P12 | 0.0640 | 0.1170 | 0.0489 | -0.0686 | -0.0197 | **Al2-P12** | 0.0638 | 0.1158 | 0.0486 | -0.0682 | -0.0196 |
| Al3-P12 | 0.0637 | 0.1169 | 0.0487 | -0.0681 | -0.0195 | **Al3-P12** | 0.0636 | 0.1156 | 0.0484 | -0.0679 | -0.0195 |
| Al3-P15 | 0.0643 | 0.1275 | 0.0509 | -0.0700 | -0.0190 | **Al3-P15** | 0.0650 | 0.1310 | 0.0520 | -0.0712 | -0.0192 |
| Al4-P13 | 0.0626 | 0.1211 | 0.0485 | -0.0668 | -0.0183 | **Al4-P13** | 0.0625 | 0.1204 | 0.0483 | -0.0665 | -0.0182 |
| Al4-P16 | 0.0658 | 0.1360 | 0.0535 | -0.0730 | -0.0195 | **Al4-P16** | 0.0610 | 0.1151 | 0.0463 | -0.0638 | -0.0175 |
| Al4-P14 | 0.0615 | 0.1156 | 0.0468 | -0.0646 | -0.0179 | **Al4-P14** | 0.0649 | 0.1256 | 0.0510 | -0.0706 | -0.0196 |
| Al5-P14 | 0.0614 | 0.1140 | 0.0464 | -0.0643 | -0.0179 | **Al5-P14** | 0.0594 | 0.1051 | 0.0435 | -0.0607 | -0.0172 |
| Al5-P17 | 0.0655 | 0.1313 | 0.0525 | -0.0721 | -0.0196 | **Al5-P17** | 0.0495 | 0.0959 | 0.0351 | -0.0463 | -0.0111 |
| Al5-P15 | 0.0625 | 0.1203 | 0.0483 | -0.0665 | -0.0182 | **Al5-P15** | 0.0597 | 0.1069 | 0.0440 | -0.0613 | -0.0173 |
| Al6-P16 | 0.0640 | 0.1314 | 0.0513 | -0.0697 | -0.0184 | **Al6-P16** | 0.0626 | 0.1225 | 0.0487 | -0.0669 | -0.0181 |
| Al6-P18 | 0.0645 | 0.1283 | 0.0512 | -0.0703 | -0.0191 | **Al6-P18** | 0.0637 | 0.1246 | 0.0500 | -0.0688 | -0.0188 |
| Al7-P16 | 0.0593 | 0.1116 | 0.0445 | -0.0611 | -0.0166 | **Al7-P16** | 0.0662 | 0.1353 | 0.0537 | -0.0735 | -0.0198 |
| Al7-P17 | 0.0602 | 0.1105 | 0.0450 | -0.0624 | -0.0174 | **Al7-P17** | 0.0595 | 0.1151 | 0.0452 | -0.0616 | -0.0164 |
| Al7-P19 | 0.0609 | 0.1146 | 0.0462 | -0.0637 | -0.0175 | **Al7-P19** | 0.0660 | 0.1315 | 0.0529 | -0.0729 | -0.0200 |
| Al8-P17 | 0.0638 | 0.1269 | 0.0504 | -0.0691 | -0.0187 | **Al8-P17** | 0.0595 | 0.1130 | 0.0448 | -0.0614 | -0.0166 |
| Al8-P20 | 0.0641 | 0.1275 | 0.0507 | -0.0696 | -0.0189 | **Al8-P20** | 0.0658 | 0.1305 | 0.0526 | -0.0725 | -0.0200 |
| Al9-P18 | 0.0627 | 0.1265 | 0.0495 | -0.0673 | -0.0179 | **Al9-P18** | 0.0636 | 0.1285 | 0.0505 | -0.0688 | -0.0184 |
| Al9-P19 | 0.0632 | 0.1294 | 0.0504 | -0.0684 | -0.0180 | **Al9-P19** | 0.0617 | 0.1207 | 0.0478 | -0.0654 | -0.0176 |
| Al10-P19 | 0.0637 | 0.1335 | 0.0514 | -0.0695 | -0.0180 | **Al10-P19** | 0.0624 | 0.1253 | 0.0491 | -0.0669 | -0.0178 |
| Al10-P20 | 0.0629 | 0.1292 | 0.0501 | -0.0678 | -0.0178 | **Al10-P20** | 0.0629 | 0.1264 | 0.0496 | -0.0676 | -0.0180 |
| P14-H63 | 0.0051 | 0.0129 | 0.0026 | -0.0019 | 0.0006 | **S61-P17** | 0.0685 | 0.0210 | 0.0365 | -0.0677 | -0.0312 |
| Se61-Al7 | 0.0356 | 0.0766 | 0.0238 | -0.0285 | -0.0047 | **O62-Al5** | 0.0676 | 0.4940 | 0.1145 | -0.1056 | 0.0090 |
| H62-Se61 | 0.1626 | -0.2011 | 0.1056 | -0.2614 | -0.1558 | **S61-O62** | 0.2220 | 0.1468 | 0.2581 | -0.4795 | -0.2214 |
| H63-Se61 | 0.1623 | -0.2084 | 0.1039 | -0.2600 | -0.1560 | **S61-O63** | 0.2702 | 1.0283 | 0.4956 | -0.7341 | -0.2385 |

**Table S3.** The bond length (in Å) of pristine AlPNT under various field strengths (in 10-3 a.u.)

|  |  |  |  |
| --- | --- | --- | --- |
| Bond/Ex | 0 | 10 | 20 |
| P11-Al1 | 2.320 | 2.319 | 2.319 |
| P11- Al2 | 2.320 | 2.319 | 2.319 |
| P12- Al2 | 2.320 | 2.319 | 2.319 |
| P12- Al3 | 2.320 | 2.319 | 2.319 |
| P13- Al1 | 2.309 | 2.310 | 2.318 |
| P13- Al4 | 2.313 | 2.312 | 2.309 |
| P14- Al2 | 2.309 | 2.310 | 2.318 |
| P14- Al4 | 2.313 | 2.312 | 2.309 |
| P14- Al5 | 2.313 | 2.312 | 2.309 |
| P15- Al3 | 2.309 | 2.310 | 2.318 |
| P15- Al5 | 2.313 | 2.312 | 2.309 |
| P16- Al4 | 2.306 | 2.307 | 2.315 |
| P16- Al6 | 2.311 | 2.310 | 2.307 |
| P16- Al7 | 2.311 | 2.310 | 2.307 |
| P17- Al5 | 2.306 | 2.307 | 2.315 |
| P17- Al7 | 2.311 | 2.310 | 2.307 |
| P17- Al8 | 2.311 | 2.310 | 2.307 |
| P18- Al6 | 2.306 | 2.307 | 2.315 |
| P18- Al9 | 2.305 | 2.302 | 2.302 |
| P19- Al7 | 2.306 | 2.307 | 2.315 |
| P19- Al9 | 2.305 | 2.302 | 2.302 |
| P19- Al10 | 2.305 | 2.302 | 2.302 |
| P20- Al10 | 2.305 | 2.302 | 2.302 |
| P20- Al8 | 2.306 | 2.307 | 2.315 |

**Table S4:** Dispersion energy values of examined complexes by calculations of the Local Molecular Orbital-Energy Decomposition Analysis (in a. u.).

|  |  |
| --- | --- |
| Complexes | Edisp |
| AlPNT/CS2 | -0.1817 |
| AlPNT/CO2 | -0.1824 |
| AlPNT/H2S | -0.1848 |
| AlPNT/H2Se | -0.1863 |
| AlPNT/SO2 | -0.1865 |