**Table 1S.** Descriptor Deﬁnitions

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| ID | Lable | Description |
| Physicochemical descriptors | | |
| 1 | qtot\_A | Total charge of A |
| 2 | qsigma\_A | σ charge of A |
| 3 | qpi\_A | π charge of A |
| 4 | pol\_A | polarizability of A |
| 5 | oensigma\_A | σ orbital-electronegativity of A |
| 6 | oenpiA | π orbital-electronegativity of A |
| 7 | pichgdens\_A | π charge density of A |
| 8 | totchgdens\_A | total charge density of A |
| 9 | qtot\_B | Total charge of B |
| 10 | qsigma\_B | σ charge of B |
| 11 | qpi\_B | π charge of B |
| 12 | pol\_B | polarizability of B |
| 13 | oensigma\_B | σ orbital-electronegativity of B |
| 14 | oenpi\_B | π orbital-electronegativity of B |
| 15 | pichgdens\_B | π charge density of B |
| 16 | totchgdens\_B | total charge density of B |
| 17 | maxqtot\_A,(Except B) | Maximum charge of A neighbors |
| 18 | minqtot\_A,( Except B) | Minimum charge of A neighbors |
| 19 | maxqtot\_B,( Except A) | Maximum charge of B neighbors |
| 20 | minqtot\_B,( Except A) | Minimum charge of B neighbors |
| 21 | maxpol\_A,( Except B) | Maximum polarizability of A neighbors |
| 22 | Minpol\_A,( Except B) | Minimum polarizability of A neighbors |
| 23 | maxpol\_B,( Except A) | Maximum polarizability of B neighbors |
| 24 | minpol\_B,( Except A) | Minimum polarizability of B neighbors |
| 25 | dqtot | Difference of total charges |
| 26 | dqsigma | Difference of σ charges |
| 27 | dqpi | Difference of π charges |
| 28 | doensigma | Difference of σ orbital-electronegativity |
| 29 | doenpi | Difference of π orbital-electronegativity |
| Topological descriptors | | |
| 30 | Hn\_A,( Except B) | number of H-atoms bonded to A |
| 31 | Cn\_A,( Except B) | number of C-atoms bonded to A |
| 32 | Nn\_A,( Except B) | number of N-atoms bonded to A |
| 33 | On\_A,( Except B) | number of O-atoms bonded to A |
| 34 | Pn\_A,( Except B) | number of P-atoms bonded to A |
| 35 | Sn\_A,( Except B) | number of S-atoms bonded to A |
| 36 | Xn\_A,( Except B) | number of halogen atoms bonded to A |
| 37 | Hn\_B,( Except A) | number of H-atoms bonded to B |
| 38 | Cn\_B,( Except A) | number of C-atoms bonded to B |
| 39 | Nn\_B,( Except A) | number of N-atoms bonded to B |
| 40 | On\_B,( Except A) | number of O-atoms bonded to B |
| 41 | Pn\_B,( Except A) | number of P-atoms bonded to B |
| 42 | Sn\_B,( Except A) | number of S-atoms bonded to B |
| 43 | Xn\_B,( Except A) | number of halogen atoms bonded to B |
| 44 | Csp1\_A | A is C sp1 |
| 45 | Csp2\_A | A is C sp2 |
| 46 | Csp3\_A | A is C sp3 |
| 47 | Csp1\_B | B is C sp1 |
| 48 | Csp2\_B | B is C sp2 |
| 49 | Csp3\_B | B is C sp3 |
| 50 | Csp1\_neigA | number of C sp1 neighbors of A |
| 51 | Csp2\_neigA | number of C sp2 neighbors of A |
| 52 | Csp3\_neigA | number of C sp3 neighbors of A |
| 53 | Csp1\_neigB | number of C sp1 neighbors of B |
| 54 | Csp2\_neigB | number of C sp2 neighbors of B |
| 55 | Csp3\_neigB | number of C sp3 neighbors of B |
| 56 | boord | bond order |

A and B are two atoms located at either end of the chemical bond.