# Supplementary information

## Elucidating the Aromatic Properties of Covalent Organic Frameworks Surface for Enhanced Polar Solvent Adsorption

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### SI.1.1. Optimization and frequency calculation

Sum of electronic and zero-point energies (hartree) used for ASE, sum of electronic and thermal enthalpies (hartree) applied for ΔH equations, and x, y, z coordinates (Å) for the optimized structures [1]:

**COF-1**

$E_0 = E_{elec} + ZPE$ = -5601.440178

$H = E + RT$ = -5601.334262

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 5 | 0 | 5.041166 | 6.341328 | 0.000000 |
| 2 | 5 | 0 | 8.012334 | 1.195113 | 0.000000 |
| 3 | 8 | 0 | 5.707193 | 7.535776 | 0.000000 |
| 4 | 8 | 0 | 9.379770 | 1.174686 | 0.000000 |
| 5 | 6 | 0 | 7.909599 | 3.768048 | 0.000000 |
| 6 | 6 | 0 | 7.229811 | 2.549671 | 0.000000 |
| 7 | 6 | 0 | 7.218025 | 4.965889 | 0.000000 |
| 8 | 6 | 0 | 5.822985 | 4.986364 | 0.000000 |
| 9 | 1 | 0 | 8.984512 | 3.773308 | 0.000000 |
| 10 | 1 | 0 | 7.760036 | 5.894161 | 0.000000 |
| 11 | 5 | 0 | 2.971169 | 7.536442 | 0.000000 |
| 12 | 8 | 0 | 3.672396 | 6.360777 | 0.000000 |
| 13 | 6 | 0 | 1.406826 | 7.536035 | 0.000000 |
| 14 | 6 | 0 | 0.691551 | 6.338153 | 0.000000 |
| 15 | 6 | 0 | -0.691551 | 6.338153 | 0.000000 |
| 16 | 6 | 0 | -1.406826 | 7.536035 | 0.000000 |
| 17 | 1 | 0 | 1.224311 | 5.404525 | 0.000000 |
| 18 | 5 | 0 | -2.971169 | 7.536442 | 0.000000 |
| 19 | 8 | 0 | -3.672396 | 6.360777 | 0.000000 |
| 20 | 1 | 0 | -1.224311 | 5.404525 | 0.000000 |
| 21 | 5 | 0 | 5.042358 | 8.733620 | 0.000000 |
| 22 | 8 | 0 | 3.672577 | 8.710462 | 0.000000 |
| 23 | 6 | 0 | 5.823110 | 10.085922 | 0.000000 |
| 24 | 6 | 0 | 5.144694 | 11.305109 | 0.000000 |
| 25 | 6 | 0 | 5.836455 | 12.503063 | 0.000000 |
| 26 | 6 | 0 | 7.231126 | 12.524677 | 0.000000 |
| 27 | 1 | 0 | 4.069579 | 11.311570 | 0.000000 |
| 28 | 5 | 0 | 8.017075 | 13.885981 | 0.000000 |
| 29 | 1 | 0 | 5.294405 | 13.431243 | 0.000000 |
| 30 | 6 | 0 | 5.143226 | 3.767977 | 0.000000 |
| 31 | 6 | 0 | 5.834777 | 2.570176 | 0.000000 |
| 32 | 1 | 0 | 4.068300 | 3.762547 | 0.000000 |
| 33 | 8 | 0 | 7.344793 | 0.000000 | 0.000000 |
| 34 | 1 | 0 | 5.292611 | 1.641978 | 0.000000 |
| 35 | 6 | 0 | 7.218164 | 10.107990 | 0.000000 |
| 36 | 6 | 0 | 7.909742 | 11.306050 | 0.000000 |
| 37 | 1 | 0 | 7.761317 | 9.180144 | 0.000000 |

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| 38 | 1 | 0 | 8.984595 | 11.300711 | 0.000000 |
| 39 | 6 | 0 | 0.691574 | 8.733937 | 0.000000 |
| 40 | 6 | 0 | -0.691574 | 8.733937 | 0.000000 |
| 41 | 1 | 0 | 1.224475 | 9.667469 | 0.000000 |
| 42 | 8 | 0 | -3.672577 | 8.710462 | 0.000000 |
| 43 | 1 | 0 | -1.224475 | 9.667469 | 0.000000 |
| 44 | 5 | 0 | -8.017075 | 13.885981 | 0.000000 |
| 45 | 6 | 0 | -7.231126 | 12.524677 | 0.000000 |
| 46 | 6 | 0 | -5.836455 | 12.503063 | 0.000000 |
| 47 | 6 | 0 | -5.144694 | 11.305109 | 0.000000 |
| 48 | 6 | 0 | -5.823110 | 10.085922 | 0.000000 |
| 49 | 1 | 0 | -5.294405 | 13.431243 | 0.000000 |
| 50 | 5 | 0 | -5.042358 | 8.733620 | 0.000000 |
| 51 | 1 | 0 | -4.069579 | 11.311570 | 0.000000 |
| 52 | 6 | 0 | -7.909742 | 11.306050 | 0.000000 |
| 53 | 6 | 0 | -7.218164 | 10.107990 | 0.000000 |
| 54 | 1 | 0 | -8.984595 | 11.300711 | 0.000000 |
| 55 | 8 | 0 | -5.707193 | 7.535776 | 0.000000 |
| 56 | 1 | 0 | -7.761317 | 9.180144 | 0.000000 |
| 57 | 5 | 0 | 10.084715 | 0.000000 | 0.000000 |
| 58 | 5 | 0 | -5.041166 | 6.341328 | 0.000000 |
| 59 | 5 | 0 | 8.012334 | -1.195113 | 0.000000 |
| 60 | 5 | 0 | 5.042358 | -8.733620 | 0.000000 |
| 61 | 5 | 0 | 8.017075 | -13.885981 | 0.000000 |
| 62 | 8 | 0 | 5.707193 | -7.535776 | 0.000000 |
| 63 | 6 | 0 | 7.909742 | -11.306050 | 0.000000 |
| 64 | 6 | 0 | 7.231126 | -12.524677 | 0.000000 |
| 65 | 6 | 0 | 7.218164 | -10.107990 | 0.000000 |
| 66 | 6 | 0 | 5.823110 | -10.085922 | 0.000000 |
| 67 | 1 | 0 | 8.984595 | -11.300711 | 0.000000 |
| 68 | 1 | 0 | 7.761317 | -9.180144 | 0.000000 |
| 69 | 5 | 0 | 2.971169 | -7.536442 | 0.000000 |
| 70 | 8 | 0 | 3.672577 | -8.710462 | 0.000000 |
| 71 | 6 | 0 | 1.406826 | -7.536035 | 0.000000 |
| 72 | 6 | 0 | 0.691574 | -8.733937 | 0.000000 |
| 73 | 6 | 0 | -0.691574 | -8.733937 | 0.000000 |
| 74 | 6 | 0 | -1.406826 | -7.536035 | 0.000000 |
| 75 | 1 | 0 | 1.224475 | -9.667469 | 0.000000 |
| 76 | 5 | 0 | -2.971169 | -7.536442 | 0.000000 |
| 77 | 8 | 0 | -3.672577 | -8.710462 | 0.000000 |
| 78 | 1 | 0 | -1.224475 | -9.667469 | 0.000000 |
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| 80 | 8 | 0 | 3.672396 | -6.360777 | 0.000000 |
| 81 | 6 | 0 | 5.822985 | -4.986364 | 0.000000 |
| 82 | 6 | 0 | 5.143226 | -3.767977 | 0.000000 |
| 83 | 6 | 0 | 5.834777 | -2.570176 | 0.000000 |
| 84 | 6 | 0 | 7.229811 | -2.549671 | 0.000000 |
| 85 | 1 | 0 | 4.068300 | -3.762547 | 0.000000 |
| 86 | 1 | 0 | 5.292611 | -1.641978 | 0.000000 |
| 87 | 6 | 0 | 5.144694 | -11.305109 | 0.000000 |

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| 88 | 6 | 0 | 5.836455 | -12.503063 | 0.000000 |
| 89 | 1 | 0 | 4.069579 | -11.311570 | 0.000000 |
| 90 | 1 | 0 | 5.294405 | -13.431243 | 0.000000 |
| 91 | 6 | 0 | 7.218025 | -4.965889 | 0.000000 |
| 92 | 6 | 0 | 7.909599 | -3.768048 | 0.000000 |
| 93 | 1 | 0 | 7.760036 | -5.894161 | 0.000000 |
| 94 | 8 | 0 | 9.379770 | -1.174686 | 0.000000 |
| 95 | 1 | 0 | 8.984512 | -3.773308 | 0.000000 |
| 96 | 6 | 0 | 0.691551 | -6.338153 | 0.000000 |
| 97 | 6 | 0 | -0.691551 | -6.338153 | 0.000000 |
| 98 | 1 | 0 | 1.224311 | -5.404525 | 0.000000 |
| 99 | 8 | 0 | -3.672396 | -6.360777 | 0.000000 |
| 100 | 1 | 0 | -1.224311 | -5.404525 | 0.000000 |
| 101 | 5 | 0 | -10.084715 | 0.000000 | 0.000000 |
| 102 | 5 | 0 | -16.034149 | 0.000000 | 0.000000 |
| 103 | 8 | 0 | -9.379770 | -1.174686 | 0.000000 |
| 104 | 6 | 0 | -13.746198 | -1.197013 | 0.000000 |
| 105 | 6 | 0 | -14.462252 | 0.000000 | 0.000000 |
| 106 | 6 | 0 | -12.362859 | -1.197118 | 0.000000 |
| 107 | 6 | 0 | -11.646220 | 0.000000 | 0.000000 |
| 108 | 1 | 0 | -14.279000 | -2.130532 | 0.000000 |
| 109 | 1 | 0 | -11.830896 | -2.131426 | 0.000000 |
| 110 | 5 | 0 | -8.012334 | 1.195113 | 0.000000 |
| 111 | 8 | 0 | -9.379770 | 1.174686 | 0.000000 |
| 112 | 6 | 0 | -7.229811 | 2.549671 | 0.000000 |
| 113 | 6 | 0 | -7.909599 | 3.768048 | 0.000000 |
| 114 | 6 | 0 | -7.218025 | 4.965889 | 0.000000 |
| 115 | 6 | 0 | -5.822985 | 4.986364 | 0.000000 |
| 116 | 1 | 0 | -8.984512 | 3.773308 | 0.000000 |
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| 118 | 5 | 0 | -8.012334 | -1.195113 | 0.000000 |
| 119 | 8 | 0 | -7.344793 | 0.000000 | 0.000000 |
| 120 | 6 | 0 | -7.229811 | -2.549671 | 0.000000 |
| 121 | 6 | 0 | -5.834777 | -2.570176 | 0.000000 |
| 122 | 6 | 0 | -5.143226 | -3.767977 | 0.000000 |
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| 124 | 1 | 0 | -5.292611 | -1.641978 | 0.000000 |
| 125 | 5 | 0 | -5.041166 | -6.341328 | 0.000000 |
| 126 | 1 | 0 | -4.068300 | -3.762547 | 0.000000 |
| 127 | 6 | 0 | -12.362859 | 1.197118 | 0.000000 |
| 128 | 6 | 0 | -13.746198 | 1.197013 | 0.000000 |
| 129 | 1 | 0 | -11.830896 | 2.131426 | 0.000000 |
| 130 | 1 | 0 | -14.279000 | 2.130532 | 0.000000 |
| 131 | 6 | 0 | -7.909599 | -3.768048 | 0.000000 |
| 132 | 6 | 0 | -7.218025 | -4.965889 | 0.000000 |
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| 134 | 8 | 0 | -5.707193 | -7.535776 | 0.000000 |
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| 137 | 6 | 0 | -5.143226 | 3.767977 | 0.000000 |

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| 138 | 1 | 0 | -5.292611 | 1.641978 | 0.000000 |
| 139 | 1 | 0 | -4.068300 | 3.762547 | 0.000000 |
| 140 | 5 | 0 | -5.042358 | -8.733620 | 0.000000 |
| 141 | 5 | 0 | -8.017075 | -13.885981 | 0.000000 |
| 142 | 6 | 0 | -7.231126 | -12.524677 | 0.000000 |
| 143 | 6 | 0 | -7.909742 | -11.306050 | 0.000000 |
| 144 | 6 | 0 | -7.218164 | -10.107990 | 0.000000 |
| 145 | 6 | 0 | -5.823110 | -10.085922 | 0.000000 |
| 146 | 1 | 0 | -8.984595 | -11.300711 | 0.000000 |
| 147 | 1 | 0 | -7.761317 | -9.180144 | 0.000000 |
| 148 | 6 | 0 | -5.836455 | -12.503063 | 0.000000 |
| 149 | 6 | 0 | -5.144694 | -11.305109 | 0.000000 |
| 150 | 1 | 0 | -5.294405 | -13.431243 | 0.000000 |
| 151 | 1 | 0 | -4.069579 | -11.311570 | 0.000000 |
| 152 | 5 | 0 | 16.034149 | 0.000000 | 0.000000 |
| 153 | 6 | 0 | 14.462252 | 0.000000 | 0.000000 |
| 154 | 6 | 0 | 13.746198 | -1.197013 | 0.000000 |
| 155 | 6 | 0 | 12.362859 | -1.197118 | 0.000000 |
| 156 | 6 | 0 | 11.646220 | 0.000000 | 0.000000 |
| 157 | 1 | 0 | 14.279000 | -2.130532 | 0.000000 |
| 158 | 1 | 0 | 11.830896 | -2.131426 | 0.000000 |
| 159 | 6 | 0 | 13.746198 | 1.197013 | 0.000000 |
| 160 | 6 | 0 | 12.362859 | 1.197118 | 0.000000 |
| 161 | 1 | 0 | 14.279000 | 2.130532 | 0.000000 |
| 162 | 1 | 0 | 11.830896 | 2.131426 | 0.000000 |
| 163 | 8 | 0 | 9.378312 | -13.850300 | 0.000000 |
| 164 | 1 | 0 | 9.822000 | -14.685439 | 0.000000 |
| 165 | 8 | 0 | 7.305556 | -15.047007 | 0.000000 |
| 166 | 1 | 0 | 7.806963 | -15.848821 | 0.000000 |
| 167 | 8 | 0 | -7.305556 | -15.047007 | 0.000000 |
| 168 | 1 | 0 | -7.806963 | -15.848821 | 0.000000 |
| 169 | 8 | 0 | -9.378312 | -13.850300 | 0.000000 |
| 170 | 1 | 0 | -9.822000 | -14.685439 | 0.000000 |
| 171 | 8 | 0 | -16.683868 | -1.196706 | 0.000000 |
| 172 | 1 | 0 | -17.628963 | -1.163382 | 0.000000 |
| 173 | 8 | 0 | -16.683868 | 1.196706 | 0.000000 |
| 174 | 1 | 0 | -17.628963 | 1.163382 | 0.000000 |
| 175 | 8 | 0 | -9.378312 | 13.850300 | 0.000000 |
| 176 | 1 | 0 | -9.822000 | 14.685439 | 0.000000 |
| 177 | 8 | 0 | -7.305556 | 15.047007 | 0.000000 |
| 178 | 1 | 0 | -7.806963 | 15.848821 | 0.000000 |
| 179 | 8 | 0 | 7.305556 | 15.047007 | 0.000000 |
| 180 | 1 | 0 | 7.806963 | 15.848821 | 0.000000 |
| 181 | 8 | 0 | 9.378312 | 13.850300 | 0.000000 |
| 182 | 1 | 0 | 9.822000 | 14.685439 | 0.000000 |
| 183 | 8 | 0 | 16.683868 | 1.196706 | 0.000000 |
| 184 | 1 | 0 | 17.628963 | 1.163382 | 0.000000 |
| 185 | 8 | 0 | 16.683868 | -1.196706 | 0.000000 |
| 186 | 1 | 0 | 17.628963 | -1.163382 | 0.000000 |

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**CTF-1**

$E_0 = E_{elec} + ZPE$ = -4969.104956

$H = E + RT$ = -4969.01747

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 7.647824 | 3.618151 | 0.000000 |
| 2 | 6 | 0 | 6.960545 | 2.408707 | 0.000000 |
| 3 | 6 | 0 | 6.957322 | 4.814135 | 0.000000 |
| 4 | 6 | 0 | 5.566274 | 4.823655 | 0.000000 |
| 5 | 1 | 0 | 8.719340 | 3.617569 | 0.000000 |
| 6 | 1 | 0 | 7.492577 | 5.742385 | 0.000000 |
| 7 | 6 | 0 | 1.394271 | 7.232362 | 0.000000 |
| 8 | 6 | 0 | 0.690510 | 6.032330 | 0.000000 |
| 9 | 6 | 0 | -0.690510 | 6.032330 | 0.000000 |
| 10 | 6 | 0 | -1.394271 | 7.232362 | 0.000000 |
| 11 | 1 | 0 | 1.227354 | 5.104957 | 0.000000 |
| 12 | 1 | 0 | -1.227354 | 5.104957 | 0.000000 |
| 13 | 6 | 0 | 5.565843 | 9.640322 | 0.000000 |
| 14 | 6 | 0 | 4.875068 | 10.848149 | 0.000000 |
| 15 | 6 | 0 | 5.562510 | 12.045973 | 0.000000 |
| 16 | 6 | 0 | 6.952111 | 12.041409 | 0.000000 |
| 17 | 1 | 0 | 3.803790 | 10.844194 | 0.000000 |
| 18 | 1 | 0 | 5.029959 | 12.978307 | 0.000000 |
| 19 | 6 | 0 | 4.878896 | 3.614164 | 0.000000 |
| 20 | 6 | 0 | 5.569405 | 2.418166 | 0.000000 |
| 21 | 1 | 0 | 3.807345 | 3.615399 | 0.000000 |
| 22 | 1 | 0 | 5.034700 | 1.489559 | 0.000000 |
| 23 | 6 | 0 | 6.957238 | 9.646007 | 0.000000 |
| 24 | 6 | 0 | 7.650864 | 10.840262 | 0.000000 |
| 25 | 1 | 0 | 7.489452 | 8.716276 | 0.000000 |
| 26 | 1 | 0 | 8.724564 | 10.845225 | 0.000000 |
| 27 | 6 | 0 | 0.690502 | 8.432285 | 0.000000 |
| 28 | 6 | 0 | -0.690502 | 8.432285 | 0.000000 |
| 29 | 1 | 0 | 1.226763 | 9.359955 | 0.000000 |
| 30 | 1 | 0 | -1.226763 | 9.359955 | 0.000000 |
| 31 | 6 | 0 | -6.952111 | 12.041409 | 0.000000 |
| 32 | 6 | 0 | -5.562510 | 12.045973 | 0.000000 |
| 33 | 6 | 0 | -4.875068 | 10.848149 | 0.000000 |
| 34 | 6 | 0 | -5.565843 | 9.640322 | 0.000000 |
| 35 | 1 | 0 | -5.029959 | 12.978307 | 0.000000 |
| 36 | 1 | 0 | -3.803790 | 10.844194 | 0.000000 |
| 37 | 6 | 0 | -7.650864 | 10.840262 | 0.000000 |
| 38 | 6 | 0 | -6.957238 | 9.646007 | 0.000000 |
| 39 | 1 | 0 | -8.724564 | 10.845225 | 0.000000 |
| 40 | 1 | 0 | -7.489452 | 8.716276 | 0.000000 |
| 41 | 6 | 0 | 7.650864 | -10.840262 | 0.000000 |

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|---|---|---|---|---|---|
| 42 | 6 | 0 | 6.952111 | -12.041409 | 0.000000 |
| 43 | 6 | 0 | 6.957238 | -9.646007 | 0.000000 |
| 44 | 6 | 0 | 5.565843 | -9.640322 | 0.000000 |
| 45 | 1 | 0 | 8.724564 | -10.845225 | 0.000000 |
| 46 | 1 | 0 | 7.489452 | -8.716276 | 0.000000 |
| 47 | 6 | 0 | 1.394271 | -7.232362 | 0.000000 |
| 48 | 6 | 0 | 0.690502 | -8.432285 | 0.000000 |
| 49 | 6 | 0 | -0.690502 | -8.432285 | 0.000000 |
| 50 | 6 | 0 | -1.394271 | -7.232362 | 0.000000 |
| 51 | 1 | 0 | 1.226763 | -9.359955 | 0.000000 |
| 52 | 1 | 0 | -1.226763 | -9.359955 | 0.000000 |
| 53 | 6 | 0 | 5.566274 | -4.823655 | 0.000000 |
| 54 | 6 | 0 | 4.878896 | -3.614164 | 0.000000 |
| 55 | 6 | 0 | 5.569405 | -2.418166 | 0.000000 |
| 56 | 6 | 0 | 6.960545 | -2.408707 | 0.000000 |
| 57 | 1 | 0 | 3.807345 | -3.615399 | 0.000000 |
| 58 | 1 | 0 | 5.034700 | -1.489559 | 0.000000 |
| 59 | 6 | 0 | 4.875068 | -10.848149 | 0.000000 |
| 60 | 6 | 0 | 5.562510 | -12.045973 | 0.000000 |
| 61 | 1 | 0 | 3.803790 | -10.844194 | 0.000000 |
| 62 | 1 | 0 | 5.029959 | -12.978307 | 0.000000 |
| 63 | 6 | 0 | 6.957322 | -4.814135 | 0.000000 |
| 64 | 6 | 0 | 7.647824 | -3.618151 | 0.000000 |
| 65 | 1 | 0 | 7.492577 | -5.742385 | 0.000000 |
| 66 | 1 | 0 | 8.719340 | -3.617569 | 0.000000 |
| 67 | 6 | 0 | 0.690510 | -6.032330 | 0.000000 |
| 68 | 6 | 0 | -0.690510 | -6.032330 | 0.000000 |
| 69 | 1 | 0 | 1.227354 | -5.104957 | 0.000000 |
| 70 | 1 | 0 | -1.227354 | -5.104957 | 0.000000 |
| 71 | 6 | 0 | -13.213374 | -1.205712 | 0.000000 |
| 72 | 6 | 0 | -13.904221 | 0.000000 | 0.000000 |
| 73 | 6 | 0 | -11.832306 | -1.202141 | 0.000000 |
| 74 | 6 | 0 | -11.131685 | 0.000000 | 0.000000 |
| 75 | 1 | 0 | -13.754523 | -2.133081 | 0.000000 |
| 76 | 1 | 0 | -11.293242 | -2.127918 | 0.000000 |
| 77 | 6 | 0 | -6.960545 | 2.408707 | 0.000000 |
| 78 | 6 | 0 | -7.647824 | 3.618151 | 0.000000 |
| 79 | 6 | 0 | -6.957322 | 4.814135 | 0.000000 |
| 80 | 6 | 0 | -5.566274 | 4.823655 | 0.000000 |
| 81 | 1 | 0 | -8.719340 | 3.617569 | 0.000000 |
| 82 | 1 | 0 | -7.492577 | 5.742385 | 0.000000 |
| 83 | 6 | 0 | -6.960545 | -2.408707 | 0.000000 |
| 84 | 6 | 0 | -5.569405 | -2.418166 | 0.000000 |
| 85 | 6 | 0 | -4.878896 | -3.614164 | 0.000000 |
| 86 | 6 | 0 | -5.566274 | -4.823655 | 0.000000 |
| 87 | 1 | 0 | -5.034700 | -1.489559 | 0.000000 |
| 88 | 1 | 0 | -3.807345 | -3.615399 | 0.000000 |
| 89 | 6 | 0 | -11.832306 | 1.202141 | 0.000000 |
| 90 | 6 | 0 | -13.213374 | 1.205712 | 0.000000 |
| 91 | 1 | 0 | -11.293242 | 2.127918 | 0.000000 |

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| 93 | 6 | 0 | -7.647824 | -3.618151 | 0.000000 |
| 94 | 6 | 0 | -6.957322 | -4.814135 | 0.000000 |
| 95 | 1 | 0 | -8.719340 | -3.617569 | 0.000000 |
| 96 | 1 | 0 | -7.492577 | -5.742385 | 0.000000 |
| 97 | 6 | 0 | -5.569405 | 2.418166 | 0.000000 |
| 98 | 6 | 0 | -4.878896 | 3.614164 | 0.000000 |
| 99 | 1 | 0 | -5.034700 | 1.489559 | 0.000000 |
| 100 | 1 | 0 | -3.807345 | 3.615399 | 0.000000 |
| 101 | 6 | 0 | -6.952111 | -12.041409 | 0.000000 |
| 102 | 6 | 0 | -7.650864 | -10.840262 | 0.000000 |
| 103 | 6 | 0 | -6.957238 | -9.646007 | 0.000000 |
| 104 | 6 | 0 | -5.565843 | -9.640322 | 0.000000 |
| 105 | 1 | 0 | -8.724564 | -10.845225 | 0.000000 |
| 106 | 1 | 0 | -7.489452 | -8.716276 | 0.000000 |
| 107 | 6 | 0 | -5.562510 | -12.045973 | 0.000000 |
| 108 | 6 | 0 | -4.875068 | -10.848149 | 0.000000 |
| 109 | 1 | 0 | -5.029959 | -12.978307 | 0.000000 |
| 110 | 1 | 0 | -3.803790 | -10.844194 | 0.000000 |
| 111 | 6 | 0 | 13.904221 | 0.000000 | 0.000000 |
| 112 | 6 | 0 | 13.213374 | -1.205712 | 0.000000 |
| 113 | 6 | 0 | 11.832306 | -1.202141 | 0.000000 |
| 114 | 6 | 0 | 11.131685 | 0.000000 | 0.000000 |
| 115 | 1 | 0 | 13.754523 | -2.133081 | 0.000000 |
| 116 | 1 | 0 | 11.293242 | -2.127918 | 0.000000 |
| 117 | 6 | 0 | 13.213374 | 1.205712 | 0.000000 |
| 118 | 6 | 0 | 11.832306 | 1.202141 | 0.000000 |
| 119 | 1 | 0 | 13.754523 | 2.133081 | 0.000000 |
| 120 | 1 | 0 | 11.293242 | 2.127918 | 0.000000 |
| 121 | 6 | 0 | 4.821473 | -8.351036 | 0.000000 |
| 122 | 6 | 0 | 4.822771 | -6.111350 | 0.000000 |
| 123 | 6 | 0 | 2.881199 | -7.232317 | 0.000000 |
| 124 | 6 | 0 | -4.821473 | -8.351036 | 0.000000 |
| 125 | 6 | 0 | -2.881199 | -7.232317 | 0.000000 |
| 126 | 6 | 0 | -4.822771 | -6.111350 | 0.000000 |
| 127 | 6 | 0 | 7.703970 | -1.120967 | 0.000000 |
| 128 | 6 | 0 | 9.642946 | 0.000000 | 0.000000 |
| 129 | 6 | 0 | 7.703970 | 1.120967 | 0.000000 |
| 130 | 6 | 0 | 4.822771 | 6.111350 | 0.000000 |
| 131 | 6 | 0 | 4.821473 | 8.351036 | 0.000000 |
| 132 | 6 | 0 | 2.881199 | 7.232317 | 0.000000 |
| 133 | 6 | 0 | -2.881199 | 7.232317 | 0.000000 |
| 134 | 6 | 0 | -4.821473 | 8.351036 | 0.000000 |
| 135 | 6 | 0 | -4.822771 | 6.111350 | 0.000000 |
| 136 | 6 | 0 | -7.703970 | 1.120967 | 0.000000 |
| 137 | 6 | 0 | -7.703970 | -1.120967 | 0.000000 |
| 138 | 6 | 0 | -9.642946 | 0.000000 | 0.000000 |
| 139 | 7 | 0 | -3.502130 | -8.399558 | 0.000000 |
| 140 | 7 | 0 | -5.523166 | -7.232713 | 0.000000 |
| 141 | 7 | 0 | -3.502328 | -6.066211 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 142 | 7 | 0 | 3.502130 | -8.399558 | 0.000000 |
| 143 | 7 | 0 | 5.523166 | -7.232713 | 0.000000 |
| 144 | 7 | 0 | 3.502328 | -6.066211 | 0.000000 |
| 145 | 7 | 0 | 9.025296 | -1.166846 | 0.000000 |
| 146 | 7 | 0 | 9.025296 | 1.166846 | 0.000000 |
| 147 | 7 | 0 | 7.004657 | 0.000000 | 0.000000 |
| 148 | 7 | 0 | 5.523166 | 7.232713 | 0.000000 |
| 149 | 7 | 0 | 3.502328 | 6.066211 | 0.000000 |
| 150 | 7 | 0 | 3.502130 | 8.399558 | 0.000000 |
| 151 | 7 | 0 | -3.502328 | 6.066211 | 0.000000 |
| 152 | 7 | 0 | -3.502130 | 8.399558 | 0.000000 |
| 153 | 7 | 0 | -5.523166 | 7.232713 | 0.000000 |
| 154 | 7 | 0 | -7.004657 | 0.000000 | 0.000000 |
| 155 | 7 | 0 | -9.025296 | -1.166846 | 0.000000 |
| 156 | 7 | 0 | -9.025296 | 1.166846 | 0.000000 |
| 157 | 6 | 0 | 7.674807 | -13.293155 | 0.000000 |
| 158 | 7 | 0 | 8.242850 | -14.277035 | 0.000000 |
| 159 | 6 | 0 | 15.349613 | 0.000000 | 0.000000 |
| 160 | 7 | 0 | 16.485700 | 0.000000 | 0.000000 |
| 161 | 6 | 0 | 7.674807 | 13.293155 | 0.000000 |
| 162 | 7 | 0 | 8.242850 | 14.277035 | 0.000000 |
| 163 | 6 | 0 | -7.674807 | 13.293155 | 0.000000 |
| 164 | 7 | 0 | -8.242850 | 14.277035 | 0.000000 |
| 165 | 6 | 0 | -15.349613 | 0.000000 | 0.000000 |
| 166 | 7 | 0 | -16.485700 | 0.000000 | 0.000000 |
| 167 | 6 | 0 | -7.674807 | -13.293155 | 0.000000 |
| 168 | 7 | 0 | -8.242850 | -14.277035 | 0.000000 |

**TPG**

$E_0 = E_{elec} + ZPE$ = -4130.252253

$H = E + RT$ = -4130.187133

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 7.877435 | 3.750554 | 0.000000 |
| 2 | 6 | 0 | 7.228035 | 2.517357 | 0.000000 |
| 3 | 6 | 0 | 7.186792 | 4.946782 | 0.000000 |
| 4 | 6 | 0 | 5.794113 | 5.000984 | 0.000000 |
| 5 | 1 | 0 | 8.947591 | 3.808568 | 0.000000 |
| 6 | 1 | 0 | 7.772112 | 5.844557 | 0.000000 |
| 7 | 6 | 0 | 1.433922 | 7.518341 | 0.000000 |
| 8 | 6 | 0 | 0.690597 | 6.339367 | 0.000000 |
| 9 | 6 | 0 | -0.690597 | 6.339367 | 0.000000 |
| 10 | 6 | 0 | -1.433922 | 7.518341 | 0.000000 |
| 11 | 1 | 0 | 1.175521 | 5.383610 | 0.000000 |
| 12 | 1 | 0 | -1.175521 | 5.383610 | 0.000000 |
| 13 | 6 | 0 | 5.796430 | 10.039711 | 0.000000 |
| 14 | 6 | 0 | 5.133866 | 11.268822 | 0.000000 |
| 15 | 6 | 0 | 5.823921 | 12.468244 | 0.000000 |
| 16 | 1 | 0 | 4.063301 | 11.315090 | 0.000000 |
| 17 | 1 | 0 | 5.273255 | 13.392062 | 0.000000 |
| 18 | 6 | 0 | 5.144754 | 3.767758 | 0.000000 |
| 19 | 6 | 0 | 5.835351 | 2.571609 | 0.000000 |
| 20 | 1 | 0 | 4.074582 | 3.709836 | 0.000000 |
| 21 | 1 | 0 | 5.250103 | 1.673774 | 0.000000 |
| 22 | 6 | 0 | 7.192153 | 10.080470 | 0.000000 |
| 23 | 6 | 0 | 7.885855 | 11.277786 | 0.000000 |
| 24 | 1 | 0 | 7.767505 | 9.176467 | 0.000000 |
| 25 | 1 | 0 | 8.961239 | 11.262804 | 0.000000 |
| 26 | 6 | 0 | 0.690642 | 8.697335 | 0.000000 |
| 27 | 6 | 0 | -0.690642 | 8.697335 | 0.000000 |
| 28 | 1 | 0 | 1.175479 | 9.653125 | 0.000000 |
| 29 | 1 | 0 | -1.175479 | 9.653125 | 0.000000 |
| 30 | 6 | 0 | -5.823921 | 12.468244 | 0.000000 |
| 31 | 6 | 0 | -5.133866 | 11.268822 | 0.000000 |
| 32 | 6 | 0 | -5.796430 | 10.039711 | 0.000000 |
| 33 | 1 | 0 | -5.273255 | 13.392062 | 0.000000 |
| 34 | 1 | 0 | -4.063301 | 11.315090 | 0.000000 |
| 35 | 6 | 0 | -7.885855 | 11.277786 | 0.000000 |
| 36 | 6 | 0 | -7.192153 | 10.080470 | 0.000000 |
| 37 | 1 | 0 | -8.961239 | 11.262804 | 0.000000 |
| 38 | 1 | 0 | -7.767505 | 9.176467 | 0.000000 |
| 39 | 6 | 0 | 7.885855 | -11.277786 | 0.000000 |
| 40 | 6 | 0 | 7.192153 | -10.080470 | 0.000000 |
| 41 | 6 | 0 | 5.796430 | -10.039711 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | 8.961239 | -11.262804 | 0.000000 |
| 43 | 1 | 0 | 7.767505 | -9.176467 | 0.000000 |
| 44 | 6 | 0 | 1.433922 | -7.518341 | 0.000000 |
| 45 | 6 | 0 | 0.690642 | -8.697335 | 0.000000 |
| 46 | 6 | 0 | -0.690642 | -8.697335 | 0.000000 |
| 47 | 6 | 0 | -1.433922 | -7.518341 | 0.000000 |
| 48 | 1 | 0 | 1.175479 | -9.653125 | 0.000000 |
| 49 | 1 | 0 | -1.175479 | -9.653125 | 0.000000 |
| 50 | 6 | 0 | 5.794113 | -5.000984 | 0.000000 |
| 51 | 6 | 0 | 5.144754 | -3.767758 | 0.000000 |
| 52 | 6 | 0 | 5.835351 | -2.571609 | 0.000000 |
| 53 | 6 | 0 | 7.228035 | -2.517357 | 0.000000 |
| 54 | 1 | 0 | 4.074582 | -3.709836 | 0.000000 |
| 55 | 1 | 0 | 5.250103 | -1.673774 | 0.000000 |
| 56 | 6 | 0 | 5.133866 | -11.268822 | 0.000000 |
| 57 | 6 | 0 | 5.823921 | -12.468244 | 0.000000 |
| 58 | 1 | 0 | 4.063301 | -11.315090 | 0.000000 |
| 59 | 1 | 0 | 5.273255 | -13.392062 | 0.000000 |
| 60 | 6 | 0 | 7.186792 | -4.946782 | 0.000000 |
| 61 | 6 | 0 | 7.877435 | -3.750554 | 0.000000 |
| 62 | 1 | 0 | 7.772112 | -5.844557 | 0.000000 |
| 63 | 1 | 0 | 8.947591 | -3.808568 | 0.000000 |
| 64 | 6 | 0 | 0.690597 | -6.339367 | 0.000000 |
| 65 | 6 | 0 | -0.690597 | -6.339367 | 0.000000 |
| 66 | 1 | 0 | 1.175521 | -5.383610 | 0.000000 |
| 67 | 1 | 0 | -1.175521 | -5.383610 | 0.000000 |
| 68 | 6 | 0 | -13.709776 | -1.190458 | 0.000000 |
| 69 | 6 | 0 | -12.326019 | -1.188353 | 0.000000 |
| 70 | 6 | 0 | -11.592859 | 0.000000 | 0.000000 |
| 71 | 1 | 0 | -14.234494 | -2.129258 | 0.000000 |
| 72 | 1 | 0 | -11.830806 | -2.138623 | 0.000000 |
| 73 | 6 | 0 | -7.228035 | 2.517357 | 0.000000 |
| 74 | 6 | 0 | -7.877435 | 3.750554 | 0.000000 |
| 75 | 6 | 0 | -7.186792 | 4.946782 | 0.000000 |
| 76 | 6 | 0 | -5.794113 | 5.000984 | 0.000000 |
| 77 | 1 | 0 | -8.947591 | 3.808568 | 0.000000 |
| 78 | 1 | 0 | -7.772112 | 5.844557 | 0.000000 |
| 79 | 6 | 0 | -7.228035 | -2.517357 | 0.000000 |
| 80 | 6 | 0 | -5.835351 | -2.571609 | 0.000000 |
| 81 | 6 | 0 | -5.144754 | -3.767758 | 0.000000 |
| 82 | 6 | 0 | -5.794113 | -5.000984 | 0.000000 |
| 83 | 1 | 0 | -5.250103 | -1.673774 | 0.000000 |
| 84 | 1 | 0 | -4.074582 | -3.709836 | 0.000000 |
| 85 | 6 | 0 | -12.326019 | 1.188353 | 0.000000 |
| 86 | 6 | 0 | -13.709776 | 1.190458 | 0.000000 |
| 87 | 1 | 0 | -11.830806 | 2.138623 | 0.000000 |
| 88 | 1 | 0 | -14.234494 | 2.129258 | 0.000000 |
| 89 | 6 | 0 | -7.877435 | -3.750554 | 0.000000 |
| 90 | 6 | 0 | -7.186792 | -4.946782 | 0.000000 |
| 91 | 1 | 0 | -8.947591 | -3.808568 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 92 | 1 | 0 | -7.772112 | -5.844557 | 0.000000 |
| 93 | 6 | 0 | -5.835351 | 2.571609 | 0.000000 |
| 94 | 6 | 0 | -5.144754 | 3.767758 | 0.000000 |
| 95 | 1 | 0 | -5.250103 | 1.673774 | 0.000000 |
| 96 | 1 | 0 | -4.074582 | 3.709836 | 0.000000 |
| 97 | 6 | 0 | -7.885855 | -11.277786 | 0.000000 |
| 98 | 6 | 0 | -7.192153 | -10.080470 | 0.000000 |
| 99 | 6 | 0 | -5.796430 | -10.039711 | 0.000000 |
| 100 | 1 | 0 | -8.961239 | -11.262804 | 0.000000 |
| 101 | 1 | 0 | -7.767505 | -9.176467 | 0.000000 |
| 102 | 6 | 0 | -5.823921 | -12.468244 | 0.000000 |
| 103 | 6 | 0 | -5.133866 | -11.268822 | 0.000000 |
| 104 | 1 | 0 | -5.273255 | -13.392062 | 0.000000 |
| 105 | 1 | 0 | -4.063301 | -11.315090 | 0.000000 |
| 106 | 6 | 0 | 13.709776 | -1.190458 | 0.000000 |
| 107 | 6 | 0 | 12.326019 | -1.188353 | 0.000000 |
| 108 | 6 | 0 | 11.592859 | 0.000000 | 0.000000 |
| 109 | 1 | 0 | 14.234494 | -2.129258 | 0.000000 |
| 110 | 1 | 0 | 11.830806 | -2.138623 | 0.000000 |
| 111 | 6 | 0 | 13.709776 | 1.190458 | 0.000000 |
| 112 | 6 | 0 | 12.326019 | 1.188353 | 0.000000 |
| 113 | 1 | 0 | 14.234494 | 2.129258 | 0.000000 |
| 114 | 1 | 0 | 11.830806 | 2.138623 | 0.000000 |
| 115 | 6 | 0 | 5.044530 | -8.737382 | 0.000000 |
| 116 | 6 | 0 | 5.043442 | -6.300351 | 0.000000 |
| 117 | 6 | 0 | 2.934543 | -7.517925 | 0.000000 |
| 118 | 6 | 0 | -5.044530 | -8.737382 | 0.000000 |
| 119 | 6 | 0 | -2.934543 | -7.517925 | 0.000000 |
| 120 | 6 | 0 | -5.043442 | -6.300351 | 0.000000 |
| 121 | 6 | 0 | 7.977985 | -1.217574 | 0.000000 |
| 122 | 6 | 0 | 10.089060 | 0.000000 | 0.000000 |
| 123 | 6 | 0 | 7.977985 | 1.217574 | 0.000000 |
| 124 | 6 | 0 | 5.043442 | 6.300351 | 0.000000 |
| 125 | 6 | 0 | 5.044530 | 8.737382 | 0.000000 |
| 126 | 6 | 0 | 2.934543 | 7.517925 | 0.000000 |
| 127 | 6 | 0 | -2.934543 | 7.517925 | 0.000000 |
| 128 | 6 | 0 | -5.044530 | 8.737382 | 0.000000 |
| 129 | 6 | 0 | -5.043442 | 6.300351 | 0.000000 |
| 130 | 6 | 0 | -7.977985 | 1.217574 | 0.000000 |
| 131 | 6 | 0 | -7.977985 | -1.217574 | 0.000000 |
| 132 | 6 | 0 | -10.089060 | 0.000000 | 0.000000 |
| 133 | 6 | 0 | 14.414475 | 0.000000 | 0.000000 |
| 134 | 1 | 0 | 15.489566 | 0.000000 | 0.000000 |
| 135 | 6 | 0 | 7.207237 | 12.483301 | 0.000000 |
| 136 | 1 | 0 | 7.744783 | 13.414358 | 0.000000 |
| 137 | 6 | 0 | -7.207237 | 12.483301 | 0.000000 |
| 138 | 1 | 0 | -7.744783 | 13.414358 | 0.000000 |
| 139 | 6 | 0 | -14.414475 | 0.000000 | 0.000000 |
| 140 | 1 | 0 | -15.489566 | 0.000000 | 0.000000 |
| 141 | 6 | 0 | -7.207237 | -12.483301 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 142 | 1 | 0 | -7.744783 | -13.414358 | 0.000000 |
| 143 | 6 | 0 | 7.207237 | -12.483301 | 0.000000 |
| 144 | 1 | 0 | 7.744783 | -13.414358 | 0.000000 |
| 145 | 6 | 0 | 9.368862 | -1.190165 | 0.000000 |
| 146 | 1 | 0 | 9.900760 | -2.114595 | 0.000000 |
| 147 | 6 | 0 | 9.368862 | 1.190165 | 0.000000 |
| 148 | 1 | 0 | 9.900760 | 2.114595 | 0.000000 |
| 149 | 6 | 0 | 7.305711 | 0.000000 | 0.000000 |
| 150 | 1 | 0 | 6.238954 | 0.000000 | 0.000000 |
| 151 | 6 | 0 | 5.715144 | 7.518589 | 0.000000 |
| 152 | 1 | 0 | 6.781673 | 7.517012 | 0.000000 |
| 153 | 6 | 0 | 3.653717 | 8.708755 | 0.000000 |
| 154 | 1 | 0 | 3.119087 | 9.631607 | 0.000000 |
| 155 | 6 | 0 | 3.652856 | 6.326931 | 0.000000 |
| 156 | 1 | 0 | 3.119477 | 5.403092 | 0.000000 |
| 157 | 6 | 0 | -3.653717 | 8.708755 | 0.000000 |
| 158 | 1 | 0 | -3.119087 | 9.631607 | 0.000000 |
| 159 | 6 | 0 | -3.652856 | 6.326931 | 0.000000 |
| 160 | 1 | 0 | -3.119477 | 5.403092 | 0.000000 |
| 161 | 6 | 0 | -5.715144 | 7.518589 | 0.000000 |
| 162 | 1 | 0 | -6.781673 | 7.517012 | 0.000000 |
| 163 | 6 | 0 | -7.305711 | 0.000000 | 0.000000 |
| 164 | 1 | 0 | -6.238954 | 0.000000 | 0.000000 |
| 165 | 6 | 0 | -9.368862 | 1.190165 | 0.000000 |
| 166 | 1 | 0 | -9.900760 | 2.114595 | 0.000000 |
| 167 | 6 | 0 | -9.368862 | -1.190165 | 0.000000 |
| 168 | 1 | 0 | -9.900760 | -2.114595 | 0.000000 |
| 169 | 6 | 0 | -3.652856 | -6.326931 | 0.000000 |
| 170 | 1 | 0 | -3.119477 | -5.403092 | 0.000000 |
| 171 | 6 | 0 | -5.715144 | -7.518589 | 0.000000 |
| 172 | 1 | 0 | -6.781673 | -7.517012 | 0.000000 |
| 173 | 6 | 0 | -3.653717 | -8.708755 | 0.000000 |
| 174 | 1 | 0 | -3.119087 | -9.631607 | 0.000000 |
| 175 | 6 | 0 | 3.653717 | -8.708755 | 0.000000 |
| 176 | 1 | 0 | 3.119087 | -9.631607 | 0.000000 |
| 177 | 6 | 0 | 5.715144 | -7.518589 | 0.000000 |
| 178 | 1 | 0 | 6.781673 | -7.517012 | 0.000000 |
| 179 | 6 | 0 | 3.652856 | -6.326931 | 0.000000 |
| 180 | 1 | 0 | 3.119477 | -5.403092 | 0.000000 |

**Benzene**

$E_0 = E_{elec} + ZPE$ = -230.595463

$H = E + RT$ = -230.590423

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 1.386175 | 0.000000 |
| 2 | 6 | 0 | 1.200463 | 0.693087 | 0.000000 |
| 3 | 1 | 0 | 0.000000 | 2.461761 | 0.000000 |
| 4 | 1 | 0 | 2.131948 | 1.230881 | 0.000000 |
| 5 | 6 | 0 | -1.200463 | -0.693087 | 0.000000 |
| 6 | 6 | 0 | 0.000000 | -1.386175 | 0.000000 |
| 7 | 1 | 0 | -2.131948 | -1.230881 | 0.000000 |
| 8 | 1 | 0 | 0.000000 | -2.461761 | 0.000000 |
| 9 | 6 | 0 | -1.200463 | 0.693087 | 0.000000 |
| 10 | 1 | 0 | -2.131948 | 1.230881 | 0.000000 |
| 11 | 6 | 0 | 1.200463 | -0.693087 | 0.000000 |
| 12 | 1 | 0 | 2.131948 | -1.230881 | 0.000000 |

**1,3,5,2,4,6-trioxatriborinane**

$E_0 = E_{elec} + ZPE$ = -300.642437

$H = E + RT$ = -300.636644

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.000000 | 1.357069 | 0.000000 |
| 2 | 8 | 0 | -1.175256 | -0.678534 | 0.000000 |
| 3 | 8 | 0 | 1.175256 | -0.678534 | 0.000000 |
| 4 | 5 | 0 | 0.000000 | -1.370901 | 0.000000 |
| 5 | 1 | 0 | 0.000000 | -2.552688 | 0.000000 |
| 6 | 5 | 0 | -1.187235 | 0.685450 | 0.000000 |
| 7 | 1 | 0 | -2.210693 | 1.276344 | 0.000000 |
| 8 | 5 | 0 | 1.187235 | 0.685450 | 0.000000 |
| 9 | 1 | 0 | 2.210693 | 1.276344 | 0.000000 |

**Phenylboronic acid**

$E_0 = E_{elec} + ZPE$ = -405.68057

$H = E + RT$ = -405.672141

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 5 | 0 | 0.000000 | 0.000000 | -1.730972 |
| 2 | 6 | 0 | 0.000000 | 0.000000 | -0.163062 |
| 3 | 6 | 0 | 0.000000 | 1.196332 | 0.554668 |
| 4 | 6 | 0 | 0.000000 | 1.200556 | 1.939621 |
| 5 | 1 | 0 | 0.000000 | 2.129732 | 0.021291 |
| 6 | 1 | 0 | 0.000000 | 2.132702 | 2.476568 |
| 7 | 6 | 0 | 0.000000 | -1.196332 | 0.554668 |
| 8 | 6 | 0 | 0.000000 | -1.200556 | 1.939621 |
| 9 | 1 | 0 | 0.000000 | -2.129732 | 0.021291 |
| 10 | 1 | 0 | 0.000000 | -2.132702 | 2.476568 |
| 11 | 8 | 0 | 0.000000 | -1.196581 | -2.383831 |
| 12 | 1 | 0 | 0.000000 | -1.159844 | -3.328650 |
| 13 | 8 | 0 | 0.000000 | 1.196581 | -2.383831 |
| 14 | 1 | 0 | 0.000000 | 1.159844 | -3.328650 |
| 15 | 6 | 0 | 0.000000 | 0.000000 | 2.632642 |
| 16 | 1 | 0 | 0.000000 | 0.000000 | 3.708786 |

**1,3,5-triazine**

$E_0 = E_{elec} + ZPE$ = -278.624669

$H = E + RT$ = -278.61989

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.172416 | 0.676895 | 0.000000 |
| 2 | 7 | 0 | -1.172416 | 0.676895 | 0.000000 |
| 3 | 7 | 0 | 0.000000 | -1.353790 | 0.000000 |
| 4 | 6 | 0 | 0.000000 | 1.279206 | 0.000000 |
| 5 | 1 | 0 | 0.000000 | 2.354192 | 0.000000 |
| 6 | 6 | 0 | -1.107825 | -0.639603 | 0.000000 |
| 7 | 1 | 0 | -2.038790 | -1.177096 | 0.000000 |
| 8 | 6 | 0 | 1.107825 | -0.639603 | 0.000000 |
| 9 | 1 | 0 | 2.038790 | -1.177096 | 0.000000 |

**Benzonitrile**

$E_0 = E_{elec} + ZPE$ = -322.332137

$H = E + RT$ = -322.325493

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 0.599164 |
| 2 | 6 | 0 | 0.000000 | 1.207009 | -0.091172 |
| 3 | 6 | 0 | 0.000000 | 1.202594 | -1.474285 |
| 4 | 1 | 0 | 0.000000 | 2.133027 | 0.453002 |
| 5 | 1 | 0 | 0.000000 | 2.133349 | -2.011221 |
| 6 | 6 | 0 | 0.000000 | -1.207009 | -0.091172 |
| 7 | 6 | 0 | 0.000000 | -1.202594 | -1.474285 |
| 8 | 1 | 0 | 0.000000 | -2.133027 | 0.453002 |
| 9 | 1 | 0 | 0.000000 | -2.133349 | -2.011221 |
| 10 | 6 | 0 | 0.000000 | 0.000000 | 2.044350 |
| 11 | 7 | 0 | 0.000000 | 0.000000 | 3.180782 |
| 12 | 6 | 0 | 0.000000 | 0.000000 | -2.164225 |
| 13 | 1 | 0 | 0.000000 | 0.000000 | -3.239288 |

**Hydrogen ($H_2$)**

$E_0 = E_{elec} + ZPE$ = -1.116243

$H = E + RT$ = -1.112938

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.000000 | 0.000000 | 0.364980 |
| 2 | 1 | 0 | 0.000000 | 0.000000 | -0.364980 |

### SI.1.2. Harmonic oscillator model of aromaticity (HOMA)

HOMA is structural based index for measuring aromaticity and it defined by Kruszewski and Krygowski [2] as following equation.

$$\mathrm{HOMA} = 1 - \frac{\alpha}{n}\sum_{i=1}^{n}\left(R_{opt} - R_i\right)^2$$

According to the equation, $\alpha$, $n$, $R_{opt}$ and $R_i$ are empirical constant, the number of bonds determined, optimal value and individual bond length, respectively. The values of $\alpha$ and $R_{opt}$ for C-C benzene ring are 257.7 and 1.388, respectively [3]. The value of $n$ is 6 since phenyl ring (ring A) has 6 bonds. The values for $R_i$ were obtained from our optimized structures which is listed in Table S1. HOMA = 1 indicates the system has all equal bond and full delocalization (benzene-like) whereas HOMA = 0 shows the system with completely localized system. Note that we were not able to measure the HOMA value of ring B since $\alpha$ and $R_{opt}$ values for B-O bond are not available.

**Table S1. The C-C bond length values for all 6 bond in ring A**

| Number | COF-1 | CTF-1 | TPG |
|---|---|---|---|
| 1 | 1.38315 | 1.38100 | 1.38128 |
| 2 | 1.39519 | 1.39108 | 1.39373 |
| 3 | 1.39518 | 1.39117 | 1.39374 |
| 4 | 1.38310 | 1.38102 | 1.38119 |
| 5 | 1.39518 | 1.39117 | 1.39374 |
| 6 | 1.39519 | 1.39108 | 1.39373 |

### SI.1.3. NICS-X-scan

The optimized structures were considered with the aim of finding aromatic property of the pore. First, COF-1, CTF-1 and TPG sheets were set perpendicular on z-axis, then ghost atoms (Bq) were situated from centre (0.0 Å) to near the pore wall (5.0 Å) with 0.1 Å distancing next each other along the x-axis [4]. Afterward, a NMR=GIAO calculation was implemented as same as optimization level and basis set, HF/6-31G(d). Consequently, isotropic values for Bq atoms (multiplied by -1) were recorded and were arranged in Table S2.

**Table S2. $NICS_{iso}$ values for COF-1, CTF-1 and TPG over the x-axis**

| Distance from centre of pore (Å) | COF-1 | CTF-1 | TPG |
|---|---|---|---|
| 5.0 | 2.0600 | 2.8316 | 2.4801 |
| 4.9 | 2.0038 | 2.7777 | 2.4549 |
| 4.8 | 1.9491 | 2.7077 | 2.4058 |
| 4.7 | 1.8959 | 2.6302 | 2.3432 |
| 4.6 | 1.8436 | 2.5502 | 2.2736 |
| 4.5 | 1.7921 | 2.4703 | 2.2005 |
| 4.4 | 1.7411 | 2.3918 | 2.1264 |
| 4.3 | 1.6906 | 2.3150 | 2.0528 |
| 4.2 | 1.6405 | 2.2398 | 1.9806 |
| 4.1 | 1.5910 | 2.1662 | 1.9106 |
| 4.0 | 1.5424 | 2.0942 | 1.8431 |
| 3.9 | 1.4949 | 2.0240 | 1.7785 |
| 3.8 | 1.4488 | 1.9557 | 1.7171 |
| 3.7 | 1.4043 | 1.8895 | 1.6588 |
| 3.6 | 1.3616 | 1.8258 | 1.6039 |
| 3.5 | 1.3208 | 1.7648 | 1.5523 |
| 3.4 | 1.2821 | 1.7067 | 1.5039 |
| 3.3 | 1.2454 | 1.6516 | 1.4586 |
| 3.2 | 1.2109 | 1.5997 | 1.4164 |
| 3.1 | 1.1785 | 1.5510 | 1.3770 |
| 3.0 | 1.1480 | 1.5054 | 1.3404 |
| 2.9 | 1.1196 | 1.4629 | 1.3064 |
| 2.8 | 1.0929 | 1.4233 | 1.2748 |
| 2.7 | 1.0681 | 1.3865 | 1.2454 |
| 2.6 | 1.0449 | 1.3523 | 1.2181 |
| 2.5 | 1.0233 | 1.3206 | 1.1927 |
| 2.4 | 1.0031 | 1.2912 | 1.1692 |
| 2.3 | 0.9843 | 1.2640 | 1.1473 |
| 2.2 | 0.9669 | 1.2388 | 1.1271 |
| 2.1 | 0.9506 | 1.2155 | 1.1082 |
| 2.0 | 0.9355 | 1.1939 | 1.0908 |

| | | | |
|---|---|---|---|
| 1.9 | 0.9215 | 1.1739 | 1.0746 |
| 1.8 | 0.9085 | 1.1555 | 1.0596 |
| 1.7 | 0.8965 | 1.1385 | 1.0458 |
| 1.6 | 0.8854 | 1.1229 | 1.0330 |
| 1.5 | 0.8752 | 1.1085 | 1.0212 |
| 1.4 | 0.8658 | 1.0953 | 1.0104 |
| 1.3 | 0.8571 | 1.0832 | 1.0005 |
| 1.2 | 0.8493 | 1.0723 | 0.9915 |
| 1.1 | 0.8422 | 1.0623 | 0.9833 |
| 1.0 | 0.8358 | 1.0534 | 0.9759 |
| 0.9 | 0.8300 | 1.0454 | 0.9694 |
| 0.8 | 0.8249 | 1.0383 | 0.9635 |
| 0.7 | 0.8205 | 1.0322 | 0.9584 |
| 0.6 | 0.8167 | 1.0269 | 0.9540 |
| 0.5 | 0.8134 | 1.0224 | 0.9503 |
| 0.4 | 0.8108 | 1.0188 | 0.9473 |
| 0.3 | 0.8088 | 1.0160 | 0.9450 |
| 0.2 | 0.8074 | 1.0140 | 0.9433 |
| 0.1 | 0.8065 | 1.0128 | 0.9423 |
| 0.0 | 0.8062 | 1.0124 | 0.9420 |

### SI.1.4. Partial atomic charges

The cluster structures used for calculation of partial atomic charges are presented in Figure S1, S2 and S3. The main parts of the solid sheets including one pore, the 6 trihedral connections resulting rings B as well as rings A were completely covered. Energy calculation using POP=Chelpg keyword was carried out at level of B3LYP with basis set of 6-31+G(d) [5]. The values for partial atomic charges obtained from electrostatic potential (EPS) fit were assigned for molecular dynamics (MD) simulations (Table S3, S4 and S5).

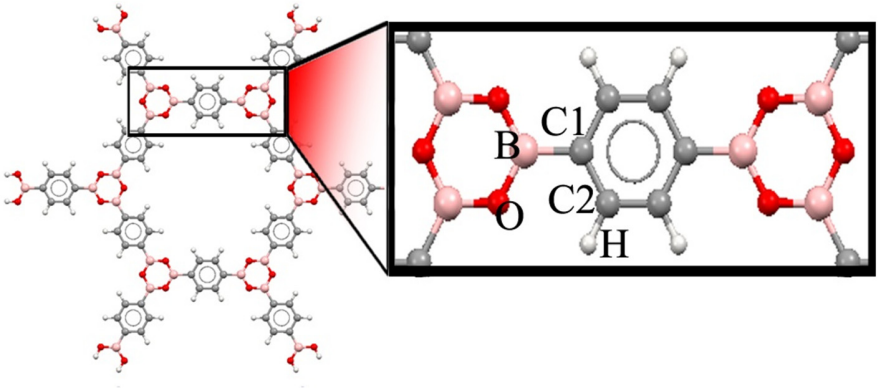


**Figure S1. COF-1 cluster structure applied for calculation of partial atomic charges. Oxygen, boron, carbon and hydrogen atoms are displayed in red, pink, gray and white spheres, respectively.**

**Table S3. Partial atomic charges values for COF-1 as given by ESP-fit based on B3LYP/6-31+G(d) method**

| **Atom** | O | B | C1 | C2 | H |
|---|---|---|---|---|---|
| **Charge (e)** | -0.7474 | 0.7793 | -0.1960 | -0.0920 | 0.1038 |

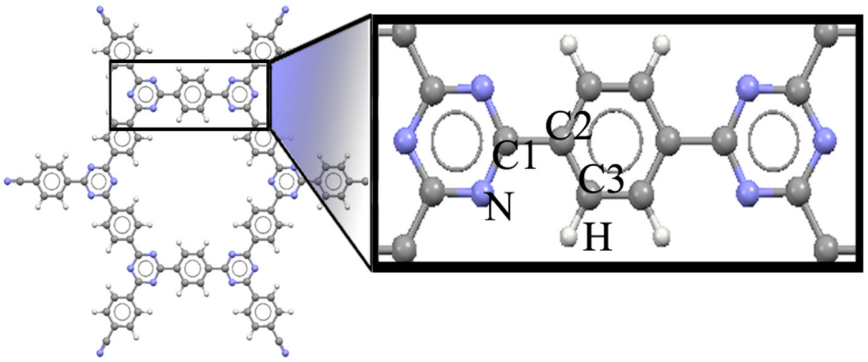


**Figure S2. CTF-1 cluster structure applied for calculation of partial atomic charges. Nitrogen, carbon and hydrogen atoms are displayed in blue, gray and white spheres, respectively.**

**Table S4. Partial atomic charges values for CTF-1 as given by ESP-fit based on B3LYP/6-31+G(d) method**

| **Atom** | N | C1 | C2 | C3 | H |
|---|---|---|---|---|---|
| **Charge (e)** | -0.6869 | 0.6486 | -0.0559 | -0.0537 | 0.1045 |

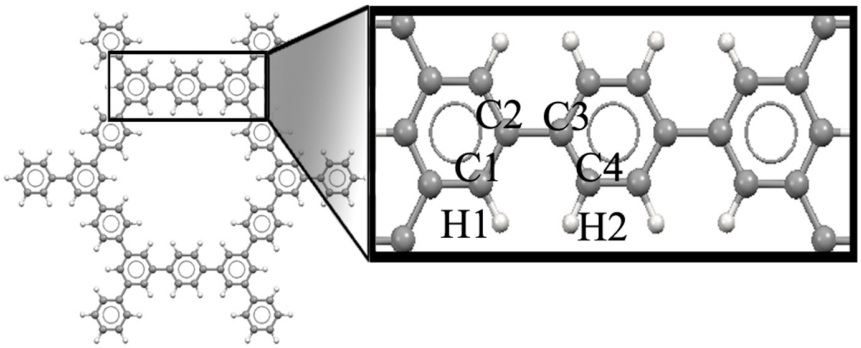


**Figure S3. TPG cluster structure applied for calculation of partial atomic charges. Carbon and hydrogen atoms are displayed in gray and white spheres, respectively**

**Table S5. Partial atomic charges values for TPG as given by ESP-fit based on B3LYP/6-31+G(d) method**

| **Atom** | C1 | C2 | C3 | C4 | H1 |
|---|---|---|---|---|---|
| **Charge (e)** | -0.1226 | 0.0298 | 0.1658 | -0.1812 | 0.0493 |
| **Atom** | H2 | | | | |
| **Charge (e)** | 0.1293 | | | | |

### SI.2.1. Super cell and unit cell of the solid sheets

2×2×1 super cell structures and the relevant unit cell for COF-1, CTF-1 and TPG are shown in Figure S4, S5, S6, respectively. However, 1×1×1 extended super cell structures have been used for this study.

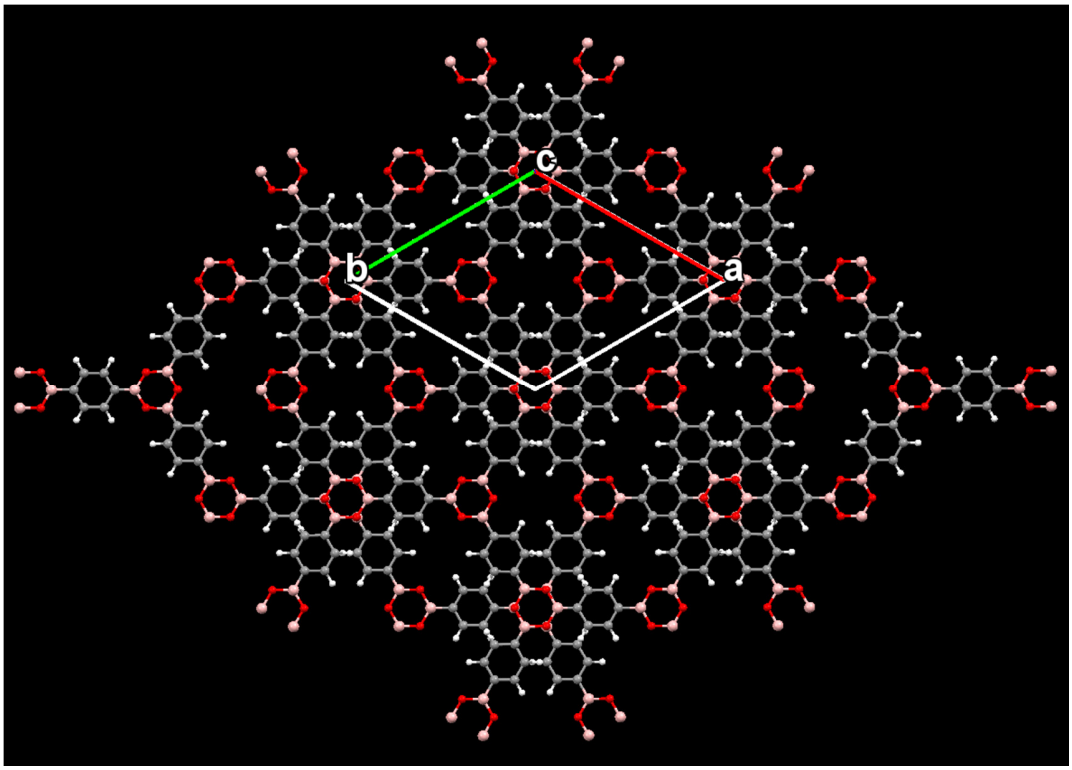


**Figure S4. 2×2×1 extended super cell for COF-1 sheet**

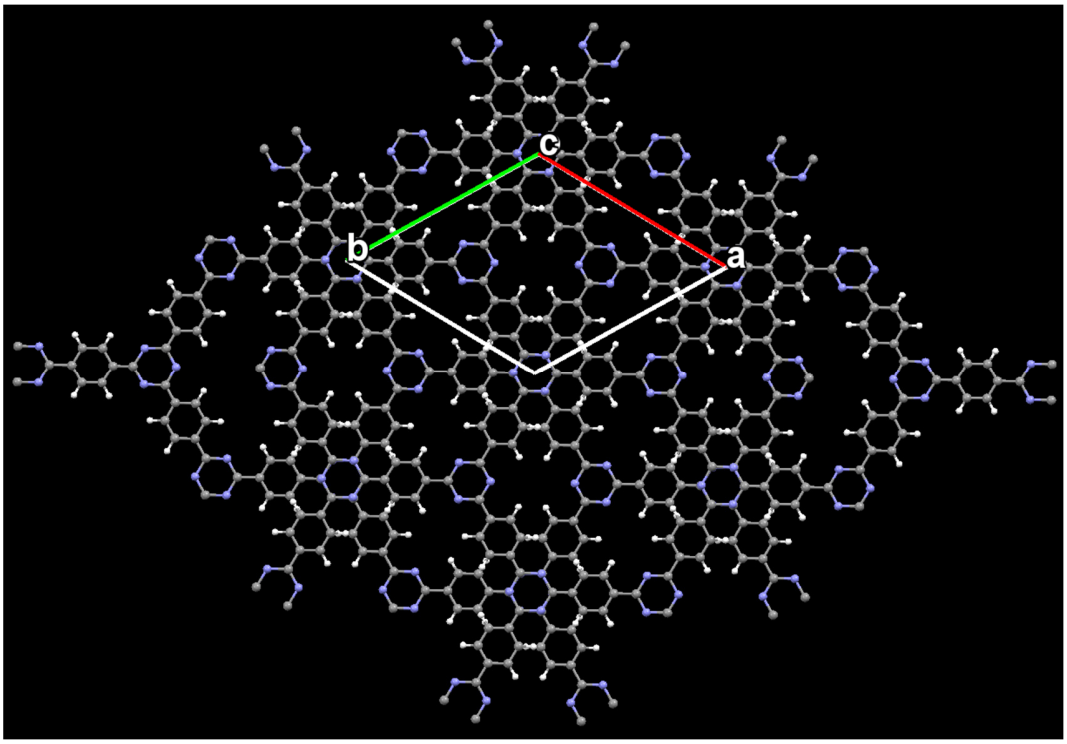


**Figure S5. 2×2×1 extended super cell for CTF-1 sheet**

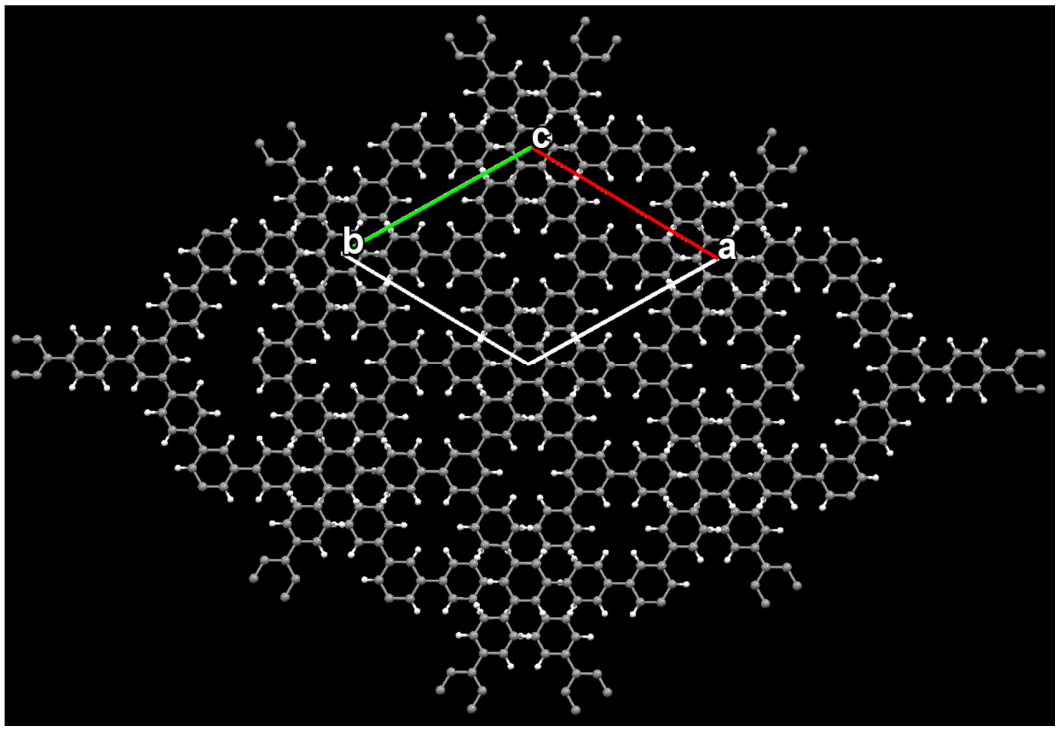


**Figure S6. 2×2×1 extended super cell for TPG sheet**

**SI.2.2. Potential parameters**

**Table S6. Lennard-Jones potential parameters for COF-1, CTF-1 and TPG taken from OBGMX web-based server derived by UFF force field [6]**

| COF | Atom type | σ (nm) | ε (kj/mol) |
|---|---|---|---|
| COF-1 | B_2 | 0.3638 | 0.7536 |
| | O_2 | 0.3118 | 0.2512 |
| | C_R | 0.3431 | 0.4396 |
| | H_ | 0.2571 | 0.1842 |
| | O_3 | 0.3118 | 0.2512 |
| CTF-1 | C_R | 0.3431 | 0.4396 |
| | C_2 | 0.3431 | 0.4396 |
| | N_R | 0.3261 | 0.2889 |
| | N_2 | 0.3261 | 0.2889 |
| | H_ | 0.2571 | 0.1842 |
| | C_3 | 0.3431 | 0.4396 |
| TPG | C_R | 0.3431 | 0.4396 |
| | C_2 | 0.3431 | 0.4396 |
| | H_ | 0.2571 | 0.1842 |
| | C_3 | 0.3431 | 0.4396 |

### SI.2.3. Total energy

Maximum number of steps for energy minimization of the systems was determined by 50000 steps. The algorithm of steepest descent minimization was applied, and the run was stopped at 30674, 50000 and 50000 steps with the potential energy of -6.43 x $10^4$, -6.60 x $10^4$ and -6.48 x $10^4$ kJ/mol for COF-1, CTF-1 and TPG, respectively. MD production of the systems was continued for 50 ns, after they were equilibrated at 300 K using NVT ensemble and at pressure of 1 bar using NPT ensemble. As plotted in Figure S7, the total energy values of the systems are not severely fluctuated, thus dynamics behavior of the water and ethanol molecules on the solid sheets can be calculated.

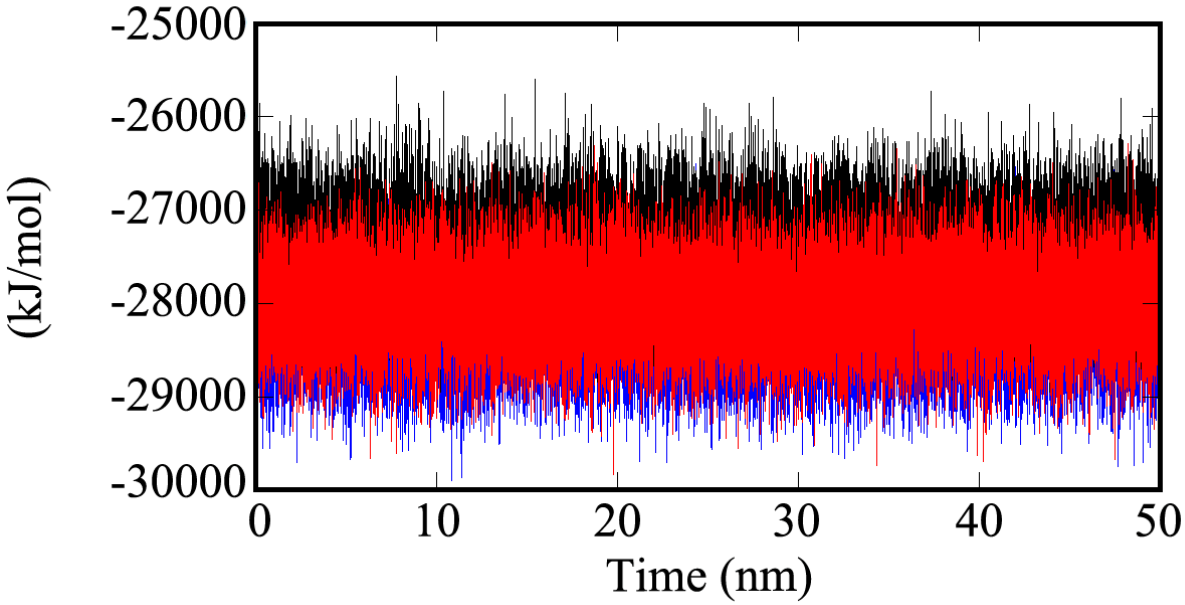


**Figure S7. Calculated total energy of the systems; red, blue and black colors are represented for COF-1, CTF-1 and TPG**

### SI.2.4. Radial distribution function (RDF)

RDF is important tool for exploring the interaction of the considered molecules with various atoms on the surface of the solid sheets [7]. The RDF, $g_{ij}$ (r), is defined as the following equation:

$$g_{ij}(r) = \frac{N_{ij}\ (r, r + \Delta r).V}{4\pi r^2.\Delta r.N_i.N_j}$$

According to the equation $N_{ij}$(r, r+Δr) is the number of atom j around atom i within the area by the distance between r and r+Δr. Also, V is indicated for the volume of system and N is the number of atoms. All the calculated RDF graphs for COF-1, CTF-1 and TPG are shown in Figure S8, S9 and S10. Also, the maximum peak value and its distance (nm) for each RDF graph can be found in Table S7.

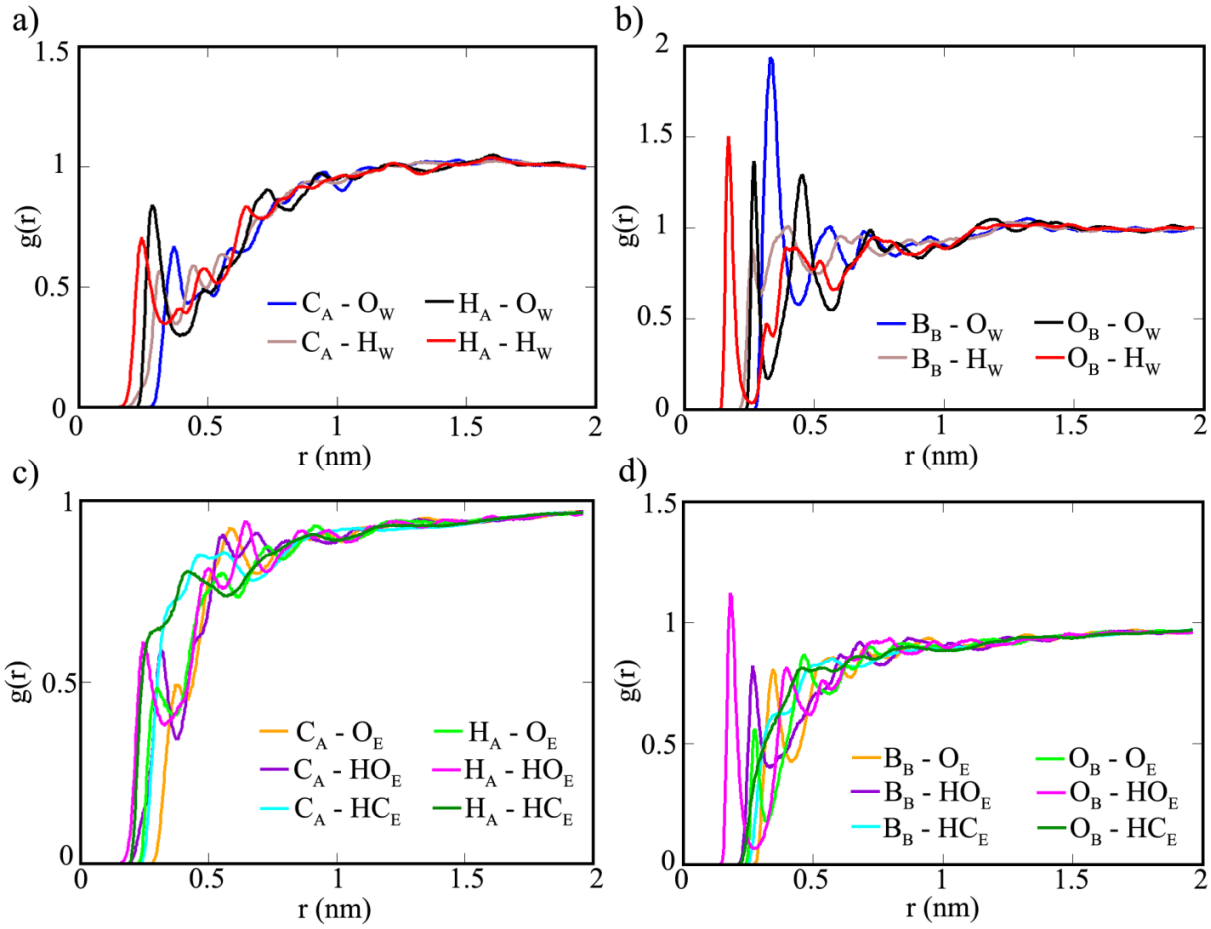


**Figure S8. RDF graphs for COF-1; a) between atoms in ring A and atoms in water, b) between atoms in ring B and atoms in water, c) between atoms in ring A and atoms in ethanol, and d) between atoms in ring B and atoms in ethanol**

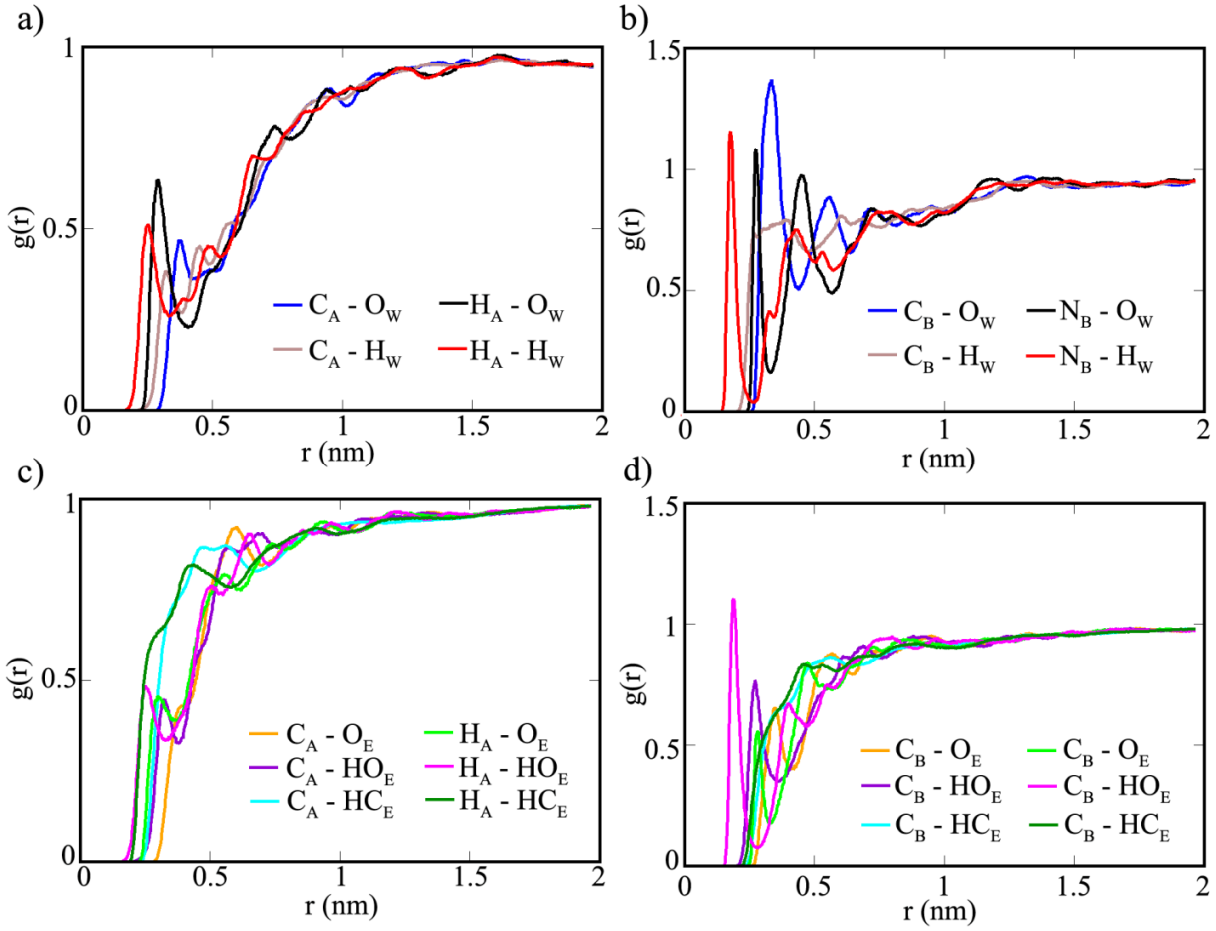


**Figure S9. RDF graphs for CTF-1; a) between atoms in ring A and atoms in water, b) between atoms in ring B and atoms in water, c) between atoms in ring A and atoms in ethanol, and d) between atoms in ring B and atoms in ethanol**

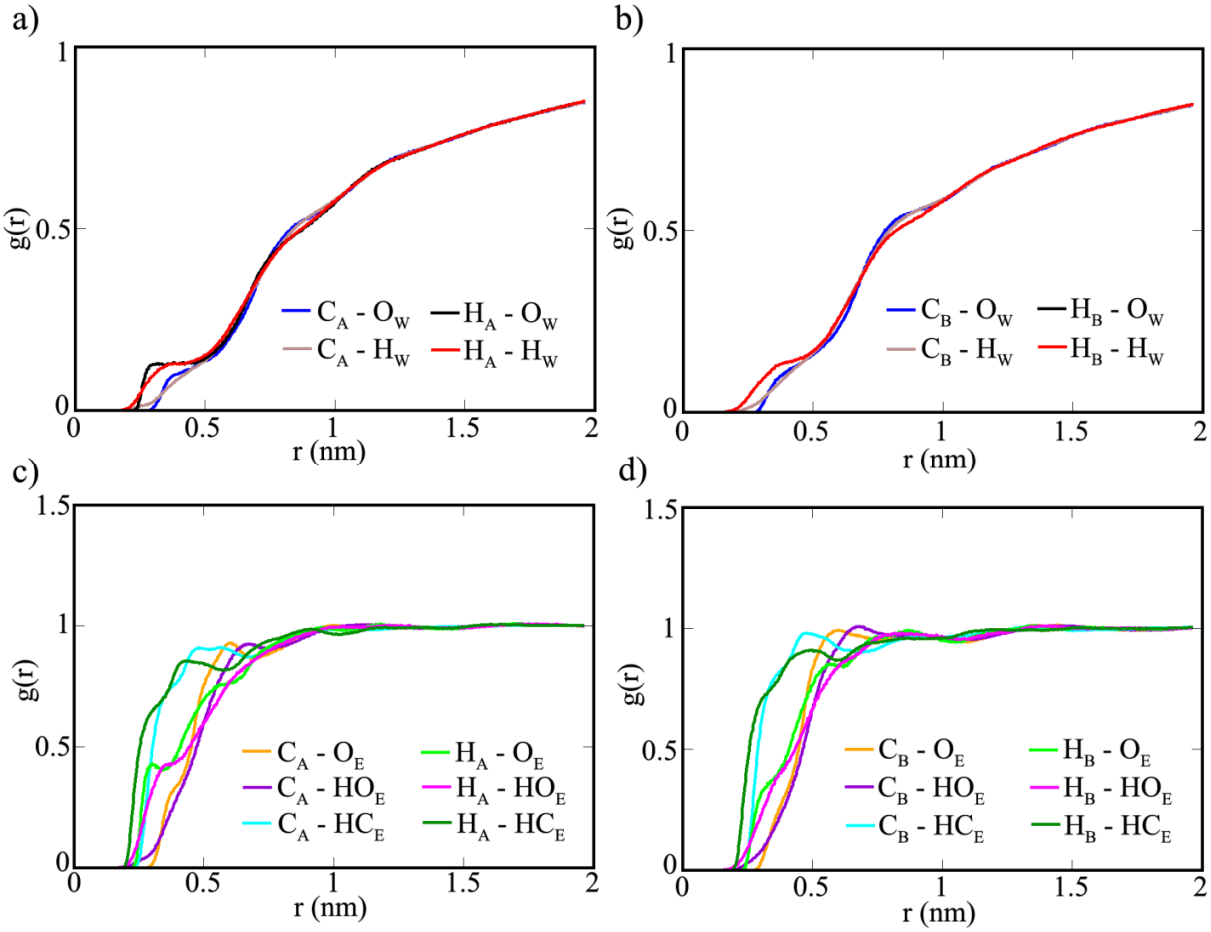


**Figure S10. RDF graphs for TPG; a) between atoms in ring A and atoms in water, b) between atoms in ring B and atoms in water, c) between atoms in ring A and atoms in ethanol, and d) between atoms in ring B and atoms in ethanol**

**Table S7. The maximum peak and its corresponding distance for each RDF**

| COF-1 | CTF-1 | TPG |
|---|---|---|
| **Ring A – water** | **Ring A – water** | **Ring A – water** |
| $C_A$ – $O_{water}$ [1.03 in 1.6 nm] | $C_A$ – $O_{water}$ [0.97 in 1.6 nm] | $C_A$ – $O_{water}$ [0.85 in 1.9 nm] |
| $C_A$ – $H_{water}$ [1.02 in 1.6 nm] | $C_A$ – $H_{water}$ [0.96 in 1.6 nm] | $C_A$ – $H_{water}$ [0.85 in 1.9 nm] |
| $H_A$ – $O_{water}$ [1.05 in 1.6 nm] | $H_A$ – $O_{water}$ [0.98 in 1.6 nm] | $H_A$ – $O_{water}$ [0.85 in 1.9 nm] |
| $H_A$ – $H_{water}$ [1.04 in 1.6 nm] | $H_A$ – $H_{water}$ [0.97 in 1.6 nm] | $H_A$ – $H_{water}$ [0.85 in 1.9 nm] |
| **Ring B – water** | **Ring B – water** | **Ring B – water** |
| $B_B$ – $O_{water}$ [1.94 in 0.3 nm] | $C_B$ – $O_{water}$ [1.37 in 0.3 nm] | $C_B$ – $O_{water}$ [0.84 in 1.9 nm] |
| $B_B$ – $H_{water}$ [1.03 in 1.2 nm] | $C_B$ – $H_{water}$ [0.95 in 1.3 nm] | $C_B$ – $H_{water}$ [0.84 in 1.9 nm] |
| $O_B$ – $O_{water}$ [1.37 in 0.3 nm] | $N_B$ – $O_{water}$ [1.08 in 0.3 nm] | $H_B$ – $O_{water}$ [0.84 in 1.9 nm] |
| $O_B$ – $H_{water}$ [1.50 in 0.2 nm] | $N_B$ – $H_{water}$ [1.15 in 0.2 nm] | $H_B$ – $H_{water}$ [0.84 in 1.9 nm] |
| **Ring A – ethanol** | **Ring A – ethanol** | **Ring A – ethanol** |
| $C_A$ – $O_{ethanol}$ [0.97 in 1.9 nm] | $C_A$ – $O_{ethanol}$ [0.98 in 1.9 nm] | $C_A$ – $O_{ethanol}$ [1.00 in 1.7 nm] |
| $C_A$ – $HO_{ethanol}$ [0.97 in 1.9 nm] | $C_A$ – $HO_{ethanol}$ [0.98 in 1.9 nm] | $C_A$ – $HO_{ethanol}$ [1.00 in 1.7 nm] |
| $C_A$ – $HC_{ethanol}$ [0.97 in 1.9 nm] | $C_A$ – $HC_{ethanol}$ [0.98 in 1.9 nm] | $C_A$ – $HC_{ethanol}$ [1.00 in 1.7-1.9 nm] |
| $H_A$ – $O_{ethanol}$ [0.97 in 1.9 nm] | $H_A$ – $O_{ethanol}$ [0.98 in 1.9 nm] | $H_A$ – $O_{ethanol}$ [1.00 in 1.7 nm] |
| $H_A$ – $HO_{ethanol}$ [0.97 in 1.8 nm] | $H_A$ – $HO_{ethanol}$ [0.98 in 1.9 nm] | $H_A$ – $HO_{ethanol}$ [1.00 in 1.7-1.8 nm] |
| $H_A$ – $HC_{ethanol}$ [0.97 in 1.9 nm] | $H_A$ – $HC_{ethanol}$ [0.98 in 1.9 nm] | $H_A$ – $HC_{ethanol}$ [1.00 in 1.6 nm] |
| **Ring B – ethanol** | **Ring B – ethanol** | **Ring B – ethanol** |
| $B_B$ – $O_{ethanol}$ [0.97 in 1.7 nm] | $C_B$ – $O_{ethanol}$ [0.98 in 1.7 nm] | $C_B$ – $O_{ethanol}$ [1.01 in 1.4 nm] |
| $B_B$ – $HO_{ethanol}$ [0.97 in 1.7 nm] | $C_B$ – $HO_{ethanol}$ [0.98 in 1.7 nm] | $C_B$ – $HO_{ethanol}$ [1.01 in 1.4 nm] |
| $B_B$ – $HC_{ethanol}$ [0.97 in 1.9 nm] | $C_B$ – $HC_{ethanol}$ [0.98 in 1.7 nm] | $C_B$ – $HC_{ethanol}$ [1.01 in 1.3 nm] |
| $O_B$ – $O_{ethanol}$ [0.97 in 1.8 nm] | $N_B$ – $O_{ethanol}$ [0.98 in 1.8 nm] | $H_B$ – $O_{ethanol}$ [1.01 in 1.3 nm] |
| $O_B$ – $HO_{ethanol}$ [1.12 in 0.2 nm] | $N_B$ – $HO_{ethanol}$ [1.10 in 0.2 nm] | $H_B$ – $HO_{ethanol}$ [1.01 in 1.3 nm] |
| $O_B$ – $HC_{ethanol}$ [0.97 in 1.9 nm] | $N_B$ – $HC_{ethanol}$ [0.98 in 1.9 nm] | $H_B$ – $HC_{ethanol}$ [1.01 in 1.9 nm] |

**SI.2.5. Average number of hydrogen bond (HB) interaction**

**Table S8.**

| Surfaces | Ring/solvent | Standard deviation | HB interaction |
|---|---|---|---|
| COF-1 | Ring A/Ethanol | 0.00 | 0.00±0.00 |
| | Ring B/Ethanol | $1.75\times10^{-2}$ | 8.70±0.28 |
| | Ring A/Water | 0.00 | 0.00±0.00 |
| | Ring B/Water | $2.17\times10^{-2}$ | 17.03±0.49 |
| CTF-1 | Ring A/Ethanol | 0.00 | 0.00±0.00 |
| | Ring B/Ethanol | $1.83\times10^{-2}$ | 9.00±0.25 |
| | Ring A/Water | 0.00 | 0.00±0.00 |
| | Ring B/Water | $2.46\times10^{-2}$ | 14.82±0.71 |
| TPG | Ring A/Ethanol | 0.00 | 0.00±0.00 |
| | Ring B/Ethanol | 0.00 | 0.00±0.00 |
| | Ring A/Water | 0.00 | 0.00±0.00 |
| | Ring B/Water | 0.00 | 0.00±0.00 |

**SI.2.6. Partial density**

**Table S9. The maximum and minimum values of partial density as well as their corresponding distance from centre of z-axis in COF-1, CTF-1 and TPG**

| Solvent | | COF-1 | CTF-1 | TPG |
|---|---|---|---|---|
| Ethanol | Max: | 748 $kg.m^{-3}$ (0.49 nm)<br>756 $kg.m^{-3}$ (-0.49 nm) | 769 $kg.m^{-3}$ (0.49 nm)<br>744 $kg.m^{-3}$ (-0.49 nm) | 832 $kg.m^{-3}$ (0.49 nm)<br>813 $kg.m^{-3}$ (-0.49 nm) |
| | Min: | 250 $kg.m^{-3}$ (0.07 nm)<br>243 $kg.m^{-3}$ (-0.07 nm) | 259 $kg.m^{-3}$ (0.07 nm)<br>259 $kg.m^{-3}$ (-0.07 nm) | 263 $kg.m^{-3}$ (0.07 nm)<br>261 $kg.m^{-3}$ (-0.07 nm) |
| Water | Max: | 265 $kg.m^{-3}$ (0.91 nm)<br>267 $kg.m^{-3}$ (-0.91 nm) | 269 $kg.m^{-3}$ (0.91 nm)<br>265 $kg.m^{-3}$ (2.89 nm) | 292 $kg.m^{-3}$ (3.43 nm)<br>290 $kg.m^{-3}$ (-3.43 nm) |
| | Min: | 153 $kg.m^{-3}$ (0.21 nm)<br>158 $kg.m^{-3}$ (-0.21 nm) | 127 $kg.m^{-3}$ (0.21 nm)<br>134 $kg.m^{-3}$ (-0.21 nm) | 35 $kg.m^{-3}$ (0.07 nm)<br>37 $kg.m^{-3}$ (-0.07 nm) |

**SI.2.7. Mean square displacement (MSD)**

**Table S10.**

| Surfaces | MSD of ethanol ($10^{-5}$ $cm^2$ $s^{-1}$) | Standard deviation | MSD of water ($10^{-5}$ $cm^2$ $s^{-1}$) | Standard deviation |
|---|---|---|---|---|
| COF-1 | 0.61±0.07 | $1.50\times10^{-1}$ | 0.80±0.01 | $1.95\times10^{-1}$ |
| CTF-1 | 0.67±0.02 | $1.64\times10^{-1}$ | 0.82±0.02 | $1.99\times10^{-1}$ |
| TPG | 0.57±0.02 | $1.40\times10^{-1}$ | 0.69±0.02 | $1.67\times10^{-1}$ |

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