

**When nanoparticle meets superhalogen: Case Study with C<sub>60</sub> fullerene**

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**Electronic supplementary information**

The atomic coordinates for the C60AlF4 equilibrium structure and the corresponding vibrational frequencies calculated using the B3LYP/6-31+G(d) method

| Coordinates (Angstroms) |           |           |           | Vibrational frequencies [cm <sup>-1</sup> ] |     |          |      |     |          |      |     |          |  |  |  |
|-------------------------|-----------|-----------|-----------|---------------------------------------------|-----|----------|------|-----|----------|------|-----|----------|--|--|--|
| Atomic Number           | x         | y         | z         | V 1                                         | (a) | 22.5573  | V 2  | (a) | 29.3148  | V 3  | (a) | 31.7385  |  |  |  |
| 6                       | -1.340951 | -3.52349  | -0.099081 | V 4                                         | (a) | 45.4356  | V 5  | (a) | 59.9481  | V 6  | (a) | 82.0427  |  |  |  |
| 6                       | 0.033657  | -3.426084 | -0.561736 | V 7                                         | (a) | 162.1114 | V 8  | (a) | 198.4701 | V 9  | (a) | 202.452  |  |  |  |
| 6                       | 1.041715  | -3.040646 | 0.321811  | V 10                                        | (a) | 261.1069 | V 11 | (a) | 262.2204 | V 12 | (a) | 264.5702 |  |  |  |
| 6                       | 0.715682  | -2.737583 | 1.705975  | V 13                                        | (a) | 265.902  | V 14 | (a) | 293.4779 | V 15 | (a) | 296.8798 |  |  |  |
| 6                       | -0.601705 | -2.831909 | 2.15004   | V 16                                        | (a) | 299.5854 | V 17 | (a) | 340.144  | V 18 | (a) | 342.6053 |  |  |  |
| 6                       | -1.653071 | -3.234397 | 1.230958  | V 19                                        | (a) | 346.4526 | V 20 | (a) | 349.0199 | V 21 | (a) | 352.9119 |  |  |  |
| 6                       | -2.20772  | -3.050583 | -1.167288 | V 22                                        | (a) | 354.1279 | V 23 | (a) | 354.9481 | V 24 | (a) | 394.1844 |  |  |  |
| 6                       | -1.367284 | -2.659894 | -2.288597 | V 25                                        | (a) | 401.1835 | V 26 | (a) | 403.7832 | V 27 | (a) | 407.817  |  |  |  |
| 6                       | 0.014518  | -2.888796 | -1.914378 | V 28                                        | (a) | 408.0941 | V 29 | (a) | 422.882  | V 30 | (a) | 428.965  |  |  |  |
| 6                       | 1.00674   | -1.991204 | -2.325524 | V 31                                        | (a) | 432.3187 | V 32 | (a) | 436.879  | V 33 | (a) | 441.5879 |  |  |  |
| 6                       | 2.067512  | -2.105845 | -0.108019 | V 34                                        | (a) | 477.072  | V 35 | (a) | 480.3319 | V 36 | (a) | 485.5053 |  |  |  |
| 6                       | 1.542776  | -1.614078 | 2.120184  | V 37                                        | (a) | 490.5067 | V 38 | (a) | 496.0327 | V 39 | (a) | 530.9052 |  |  |  |
| 6                       | 1.017334  | -0.630856 | 2.969734  | V 40                                        | (a) | 535.8672 | V 41 | (a) | 537.6925 | V 42 | (a) | 539.4099 |  |  |  |
| 6                       | -0.342936 | -0.730164 | 3.437229  | V 43                                        | (a) | 540.4122 | V 44 | (a) | 541.2159 | V 45 | (a) | 542.9742 |  |  |  |
| 6                       | -1.144161 | -1.806169 | 3.030626  | V 46                                        | (a) | 544.2933 | V 47 | (a) | 563.4087 | V 48 | (a) | 564.9393 |  |  |  |
| 6                       | -2.524933 | -1.579754 | 2.66139   | V 49                                        | (a) | 566.3341 | V 50 | (a) | 572.6648 | V 51 | (a) | 574.9226 |  |  |  |
| 6                       | -2.843173 | -2.459877 | 1.546349  | V 52                                        | (a) | 575.718  | V 53 | (a) | 576.2242 | V 54 | (a) | 576.8159 |  |  |  |
| 6                       | -3.675167 | -2.009254 | 0.522322  | V 55                                        | (a) | 577.9262 | V 56 | (a) | 582.0864 | V 57 | (a) | 585.7074 |  |  |  |
| 6                       | -3.350762 | -2.310674 | -0.863653 | V 58                                        | (a) | 587.7259 | V 59 | (a) | 589.7515 | V 60 | (a) | 607.2132 |  |  |  |
| 6                       | -1.70623  | -1.54435  | -3.061902 | V 61                                        | (a) | 676.0591 | V 62 | (a) | 676.5166 | V 63 | (a) | 676.6186 |  |  |  |
| 6                       | -2.891445 | -0.77963  | -2.74279  | V 64                                        | (a) | 676.741  | V 65 | (a) | 678.9281 | V 66 | (a) | 697.7189 |  |  |  |
| 6                       | -3.699762 | -1.151016 | -1.667137 | V 67                                        | (a) | 699.9626 | V 68 | (a) | 701.4534 | V 69 | (a) | 708.0267 |  |  |  |
| 6                       | -4.232166 | -0.134896 | -0.778357 | V 70                                        | (a) | 717.9177 | V 71 | (a) | 719.4228 | V 72 | (a) | 722.2586 |  |  |  |
| 6                       | -4.22381  | -0.662862 | 0.571173  | V 73                                        | (a) | 724.334  | V 74 | (a) | 727.9555 | V 75 | (a) | 737.475  |  |  |  |
| 6                       | -3.919687 | 0.179836  | 1.644239  | V 76                                        | (a) | 740.2216 | V 77 | (a) | 740.6817 | V 78 | (a) | 740.8667 |  |  |  |
| 6                       | -3.056302 | -0.285076 | 2.707449  | V 79                                        | (a) | 742.9446 | V 80 | (a) | 744.5699 | V 81 | (a) | 746.7148 |  |  |  |
| 6                       | -2.226485 | 0.833641  | 3.13483   | V 82                                        | (a) | 748.0441 | V 83 | (a) | 749.4201 | V 84 | (a) | 749.9391 |  |  |  |
| 6                       | -0.899346 | 0.616184  | 3.490057  | V 85                                        | (a) | 750.7037 | V 86 | (a) | 752.0128 | V 87 | (a) | 756.4858 |  |  |  |

The atomic coordinates for the C60MgF3 equilibrium structure and the corresponding vibrational frequencies calculated using the B3LYP/6-31+G(d) method

| Coordinates (Angstroms) |           |           |           | Vibrational frequencies [cm <sup>-1</sup> ] |           |            |           |            |           |
|-------------------------|-----------|-----------|-----------|---------------------------------------------|-----------|------------|-----------|------------|-----------|
| Atomic Number           | x         | y         | z         |                                             |           |            |           |            |           |
| 6                       | -3.263094 | -0.712249 | 1.423314  | V 1 (a")                                    | 14.5391   | V 2 (a")   | 20.6787   | V 3 (a')   | 44.0507   |
| 6                       | -2.416350 | -0.851125 | 2.598623  | V 4 (a')                                    | 96.4874   | V 5 (a')   | 105.6705  | V 6 (a")   | 163.3104  |
| 6                       | -1.629111 | 0.227907  | 3.022544  | V 7 (a)                                     | 202.5284  | V 8 (a)    | 202.5728  | V 9 (a")   | 249.356   |
| 6                       | -1.658284 | 1.479002  | 2.301295  | V 10 (a')                                   | 255.1642  | V 11 (a')  | 259.1539  | V 12 (a")  | 264.8906  |
| 6                       | -2.462361 | 1.610902  | 1.161592  | V 13 (a')                                   | 266.6058  | V 14 (a')  | 311.6402  | V 15 (a')  | 336.6666  |
| 6                       | -3.289049 | 0.493102  | 0.723952  | V 16 (a")                                   | 344.1918  | V 17 (a")  | 347.0858  | V 18 (a')  | 352.7755  |
| 6                       | -3.237694 | -1.971126 | 0.698516  | V 19 (a')                                   | 357.8346  | V 20 (a")  | 358.3494  | V 21 (a')  | 365.1633  |
| 6                       | -2.374474 | -2.887754 | 1.425947  | V 22 (a')                                   | 394.2224  | V 23 (a")  | 399.4886  | V 24 (a')  | 406.3671  |
| 6                       | -1.869290 | -2.193012 | 2.601088  | V 25 (a")                                   | 407.4964  | V 26 (a")  | 408.8076  | V 27 (a')  | 415.974   |
| 6                       | -0.555877 | -2.411605 | 3.030397  | V 28 (a")                                   | 428.5086  | V 29 (a')  | 435.3495  | V 30 (a")  | 437.5958  |
| 6                       | -0.263617 | -0.002281 | 3.469753  | V 31 (a')                                   | 441.4357  | V 32 (a')  | 445.9425  | V 33 (a")  | 477.4523  |
| 6                       | -0.296147 | 2.030759  | 2.292141  | V 34 (a)                                    | 488.015   | V 35 (a)   | 488.0457  | V 36 (a')  | 490.8668  |
| 6                       | 0.192221  | 2.709290  | 1.186961  | V 37 (a')                                   | 493.3758  | V 38 (a')  | 530.7352  | V 39 (a")  | 531.8764  |
| 6                       | -0.687667 | 3.021984  | 0.000000  | V 40 (a")                                   | 535.2238  | V 41 (a')  | 536.3379  | V 42 (a")  | 539.5542  |
| 6                       | -1.984997 | 2.303341  | 0.000000  | V 43 (a')                                   | 540.9063  | V 44 (a")  | 541.6311  | V 45 (a')  | 542.2801  |
| 6                       | -2.462361 | 1.610902  | -1.161592 | V 46 (a')                                   | 559.3848  | V 47 (a")  | 562.5204  | V 48 (a')  | 565.8602  |
| 6                       | -3.289049 | 0.493102  | -0.723952 | V 49 (a")                                   | 568.7831  | V 50 (a')  | 570.8933  | V 51 (a")  | 573.5497  |
| 6                       | -3.263094 | -0.712249 | -1.423314 | V 52 (a")                                   | 575.6196  | V 53 (a")  | 578.0353  | V 54 (a')  | 579.525   |
| 6                       | -3.237694 | -1.971126 | -0.698516 | V 55 (a")                                   | 580.9634  | V 56 (a")  | 582.123   | V 57 (a')  | 585.4451  |
| 6                       | -1.546110 | -3.766241 | 0.727558  | V 58 (a')                                   | 593.389   | V 59 (a")  | 593.7834  | V 60 (a')  | 673.7181  |
| 6                       | -1.546110 | -3.766241 | -0.727558 | V 61 (a")                                   | 675.9114  | V 62 (a")  | 678.846   | V 63 (a')  | 678.9524  |
| 6                       | -2.374474 | -2.887754 | -1.425947 | V 64 (a")                                   | 683.4337  | V 65 (a')  | 709.621   | V 66 (a")  | 713.7908  |
| 6                       | -1.869290 | -2.193012 | -2.601088 | V 67 (a')                                   | 715.9439  | V 68 (a")  | 718.1852  | V 69 (a')  | 718.3611  |
| 6                       | -2.416350 | -0.851125 | -2.598623 | V 70 (a')                                   | 723.4086  | V 71 (a')  | 724.4329  | V 72 (a")  | 726.4857  |
| 6                       | -1.629111 | 0.227907  | -3.022544 | V 73 (a")                                   | 737.585   | V 74 (a')  | 740.0101  | V 75 (a")  | 741.3102  |
| 6                       | -1.658284 | 1.479002  | -2.301295 | V 76 (a')                                   | 742.4476  | V 77 (a')  | 742.9506  | V 78 (a")  | 745.783   |
| 6                       | -0.296147 | 2.030759  | -2.292141 | V 79 (a)                                    | 750.0453  | V 80 (a)   | 750.0655  | V 81 (a")  | 752.2481  |
| 6                       | 0.192221  | 2.709290  | -1.186961 | V 82 (a')                                   | 753.04    | V 83 (a")  | 754.0564  | V 84 (a')  | 756.7166  |
| 6                       | 0.554474  | 1.113946  | 3.020817  | V 85 (a")                                   | 757.8438  | V 86 (a')  | 758.4854  | V 87 (a")  | 761.1971  |
| 6                       | 3.229360  | 0.659385  | -0.698295 | V 88 (a')                                   | 764.1064  | V 89 (a")  | 767.999   | V 90 (a')  | 768.9077  |
| 6                       | 3.229360  | 0.659385  | 0.698295  | V 91 (a')                                   | 772.6469  | V 92 (a")  | 772.7191  | V 93 (a")  | 780.7376  |
| 6                       | 3.258148  | -0.597296 | 1.424069  | V 94 (a')                                   | 784.4792  | V 95 (a')  | 788.3155  | V 96 (a')  | 791.9652  |
| 6                       | 3.282883  | -1.807853 | 0.726472  | V 97 (a")                                   | 793.0121  | V 98 (a")  | 805.9878  | V 99 (a')  | 806.2717  |
| 6                       | 3.282883  | -1.807853 | -0.726472 | V 100 (a")                                  | 806.454   | V 101 (a') | 814.7883  | V 102 (a") | 839.6891  |
| 6                       | 2.413516  | -0.453998 | -2.600138 | V 103 (a')                                  | 841.9653  | V 104 (a") | 843.5953  | V 105 (a') | 965.3444  |
| 6                       | 1.868108  | 0.892571  | -2.597196 | V 106 (a')                                  | 967.8735  | V 107 (a") | 973.7578  | V 108 (a') | 976.0932  |
| 6                       | 2.369693  | 1.579289  | -1.426143 | V 109 (a")                                  | 976.3341  | V 110 (a') | 981.1033  | V 111 (a') | 984.1014  |
| 6                       | 1.531087  | 2.451498  | -0.728070 | V 112 (a")                                  | 987.4528  | V 113 (a") | 1086.8138 | V 114 (a') | 1092.9896 |
| 6                       | 1.531087  | 2.451498  | 0.728070  | V 115 (a')                                  | 1099.7252 | V 116 (a") | 1102.2495 | V 117 (a') | 1109.8275 |
| 6                       | 2.369693  | 1.579289  | 1.426143  | V 118 (a')                                  | 1118.3896 | V 119 (a") | 1122.2641 | V 120 (a') | 1124.7006 |
| 6                       | 2.413516  | -0.453998 | 2.600138  | V 121 (a")                                  | 1126.7329 | V 122 (a") | 1185.7944 | V 123 (a') | 1186.937  |
| 6                       | 1.626085  | -1.524689 | 3.029022  | V 124 (a')                                  | 1200.1111 | V 125 (a') | 1205.5612 | V 126 (a') | 1209.5189 |
| 6                       | 1.651454  | -2.780731 | 2.304659  | V 127 (a")                                  | 1209.8714 | V 128 (a') | 1220.3275 | V 129 (a") | 1230.0068 |
| 6                       | 2.463133  | -2.920405 | 1.174879  | V 130 (a")                                  | 1239.4227 | V 131 (a') | 1242.6326 | V 132 (a") | 1243.3923 |
| 6                       | 1.957293  | -3.608324 | 0.000000  | V 133 (a")                                  | 1264.0397 | V 134 (a') | 1267.3241 | V 135 (a") | 1269.7039 |
| 6                       | 2.463133  | -2.920405 | -1.174879 | V 136 (a')                                  | 1272.0757 | V 137 (a') | 1282.138  | V 138 (a") | 1295.8678 |
| 6                       | 1.651454  | -2.780731 | -2.304659 | V 139 (a')                                  | 1299.0232 | V 140 (a") | 1306.0356 | V 141 (a") | 1318.6217 |
| 6                       | 1.626085  | -1.524689 | -3.029022 | V 142 (a")                                  | 1323.693  | V 143 (a') | 1328.6662 | V 144 (a') | 1333.7724 |
| 6                       | 0.554474  | 1.113946  | -3.020817 | V 145 (a")                                  | 1333.9262 | V 146 (a') | 1336.2412 | V 147 (a') | 1338.2228 |
| 6                       | -0.263617 | -0.002281 | -3.469753 | V 148 (a")                                  | 1338.8588 | V 149 (a") | 1352.6624 | V 150 (a') | 1362.6898 |
| 6                       | 0.260204  | -1.293678 | -3.477551 | V 151 (a")                                  | 1367.9294 | V 152 (a") | 1369.7856 | V 153 (a") | 1371.9256 |
| 6                       | -0.555877 | -2.411605 | -3.030397 | V 154 (a')                                  | 1372.0197 | V 155 (a") | 1378.75   | V 156 (a') | 1380.6128 |
| 6                       | 0.301797  | -3.328822 | -2.304485 | V 157 (a")                                  | 1409.7997 | V 158 (a') | 1418.0166 | V 159 (a") | 1436.0169 |
| 6                       | -0.181622 | -3.993694 | -1.175544 | V 160 (a')                                  | 1443.2944 | V 161 (a") | 1451.1876 | V 162 (a') | 1451.2159 |
| 6                       | 0.659825  | -4.131491 | 0.000000  | V 163 (a')                                  | 1455.057  | V 164 (a") | 1457.5558 | V 165 (a') | 1459.5888 |
| 6                       | -0.181622 | -3.993694 | 1.175544  | V 166 (a')                                  | 1462.7987 | V 167 (a") | 1463.2913 | V 168 (a') | 1465.4184 |
| 6                       | 0.301797  | -3.328822 | 2.304485  | V 169 (a')                                  | 1497.036  | V 170 (a") | 1508.5773 | V 171 (a") | 1519.041  |
| 6                       | 1.868108  | 0.892571  | 2.597196  | V 172 (a')                                  | 1532.7845 | V 173 (a") | 1541.0932 | V 174 (a') | 1550.2748 |
| 6                       | 0.260204  | -1.293678 | 3.477551  | V 175 (a')                                  | 1558.2865 | V 176 (a") | 1563.4782 | V 177 (a') | 1577.6838 |
| 6                       | 3.258148  | -0.597296 | -1.424069 | V 178 (a")                                  | 1597.5771 | V 179 (a') | 1600.6801 | V 180 (a") | 1601.1263 |
| 12                      | 0.136372  | 6.183906  | 0.000000  | V 181 (a')                                  | 1603.8289 | V 182 (a") | 1604.6753 | V 183 (a") | 1605.7566 |
| 9                       | -1.032580 | 4.560254  | 0.000000  | V 184 (a')                                  | 1609.7747 | V 185 (a") | 1609.9317 | V 186 (a') | 1612.8675 |
| 9                       | -0.835628 | 7.678742  | 0.000000  |                                             |           |            |           |            |           |
| 9                       | 1.777971  | 5.457331  | 0.000000  |                                             |           |            |           |            |           |

The atomic coordinates for the C60LiF2 equilibrium structure and the corresponding vibrational frequencies calculated using the B3LYP/6-31+G(d) method

| Atomic Number | Coordinates (Angstroms) |           |           | Vibrational frequencies [cm <sup>-1</sup> ] |     |       |     |       |     |
|---------------|-------------------------|-----------|-----------|---------------------------------------------|-----|-------|-----|-------|-----|
|               | x                       | y         | z         | V 1                                         | (a) | V 2   | (a) | V 3   | (a) |
| 6             | -1.591364               | -2.770724 | -1.083857 | V 4                                         | (a) | V 5   | (a) | V 6   | (a) |
| 6             | -1.486355               | -1.982973 | -2.321556 | V 7                                         | (a) | V 8   | (a) | V 9   | (a) |
| 6             | -0.133139               | -2.102686 | -2.812760 | V 10                                        | (a) | V 11  | (a) | V 12  | (a) |
| 6             | 0.604097                | -2.963872 | -1.900020 | V 13                                        | (a) | V 14  | (a) | V 15  | (a) |
| 6             | -0.299503               | -3.376510 | -0.837886 | V 16                                        | (a) | V 17  | (a) | V 18  | (a) |
| 6             | 1.942463                | -2.698947 | -1.613071 | V 19                                        | (a) | V 20  | (a) | V 21  | (a) |
| 6             | 2.602142                | -1.553655 | -2.220630 | V 22                                        | (a) | V 23  | (a) | V 24  | (a) |
| 6             | 1.895594                | -0.723595 | -3.097096 | V 25                                        | (a) | V 26  | (a) | V 27  | (a) |
| 6             | 0.506644                | -1.003619 | -3.402662 | V 28                                        | (a) | V 29  | (a) | V 30  | (a) |
| 6             | 3.492661                | -0.975471 | -1.232070 | V 31                                        | (a) | V 32  | (a) | V 33  | (a) |
| 6             | 3.646338                | 0.410360  | -1.154537 | V 34                                        | (a) | V 35  | (a) | V 36  | (a) |
| 6             | 2.913272                | 1.274665  | -2.065680 | V 37                                        | (a) | V 38  | (a) | V 39  | (a) |
| 6             | 2.057732                | 0.720822  | -3.018638 | V 40                                        | (a) | V 41  | (a) | V 42  | (a) |
| 6             | -0.194019               | 0.266359  | -3.513526 | V 43                                        | (a) | V 44  | (a) | V 45  | (a) |
| 6             | 0.764426                | 1.332932  | -3.277480 | V 46                                        | (a) | V 47  | (a) | V 48  | (a) |
| 6             | 0.377458                | 2.473465  | -2.569485 | V 49                                        | (a) | V 50  | (a) | V 51  | (a) |
| 6             | 1.268853                | 3.049355  | -1.575120 | V 52                                        | (a) | V 53  | (a) | V 54  | (a) |
| 6             | 2.510554                | 2.462948  | -1.329177 | V 55                                        | (a) | V 56  | (a) | V 57  | (a) |
| 6             | 2.996664                | 2.331817  | 0.035105  | V 58                                        | (a) | V 59  | (a) | V 60  | (a) |
| 6             | 3.695604                | 1.063285  | 0.142137  | V 61                                        | (a) | V 62  | (a) | V 63  | (a) |
| 6             | 3.599504                | 0.304818  | 1.313698  | V 64                                        | (a) | V 65  | (a) | V 66  | (a) |
| 6             | 3.443402                | -1.137192 | 1.234321  | V 67                                        | (a) | V 68  | (a) | V 69  | (a) |
| 6             | 3.388594                | -1.765628 | -0.013442 | V 70                                        | (a) | V 71  | (a) | V 72  | (a) |
| 6             | 2.432648                | -2.830501 | -0.248626 | V 73                                        | (a) | V 74  | (a) | V 75  | (a) |
| 6             | 2.217098                | 2.789587  | 1.100108  | V 76                                        | (a) | V 77  | (a) | V 78  | (a) |
| 6             | 0.924927                | 3.398463  | 0.847421  | V 79                                        | (a) | V 80  | (a) | V 81  | (a) |
| 6             | 0.456157                | 3.524148  | -0.464484 | V 82                                        | (a) | V 83  | (a) | V 84  | (a) |
| 6             | -0.931956               | 3.243322  | -0.770657 | V 85                                        | (a) | V 86  | (a) | V 87  | (a) |
| 6             | -0.982109               | 2.592548  | -2.071042 | V 88                                        | (a) | V 89  | (a) | V 90  | (a) |
| 6             | -1.897318               | 1.566737  | -2.297862 | V 91                                        | (a) | V 92  | (a) | V 93  | (a) |
| 6             | -1.497290               | 0.385093  | -3.032686 | V 94                                        | (a) | V 95  | (a) | V 96  | (a) |
| 6             | -2.156872               | -0.757520 | -2.412646 | V 97                                        | (a) | V 98  | (a) | V 99  | (a) |
| 6             | 2.113300                | 1.999083  | 2.318618  | V 100                                       | (a) | V 101 | (a) | V 102 | (a) |
| 6             | 2.794179                | 0.782475  | 2.424126  | V 103                                       | (a) | V 104 | (a) | V 105 | (a) |
| 6             | 2.141750                | -0.363937 | 3.033000  | V 106                                       | (a) | V 107 | (a) | V 108 | (a) |
| 6             | 2.543268                | -1.551473 | 2.296636  | V 109                                       | (a) | V 110 | (a) | V 111 | (a) |
| 6             | 1.621929                | -2.577035 | 2.069685  | V 112                                       | (a) | V 113 | (a) | V 114 | (a) |
| 6             | 1.566968                | -3.231239 | 0.771949  | V 115                                       | (a) | V 116 | (a) | V 117 | (a) |
| 6             | 0.173483                | -3.511614 | 0.470950  | V 118                                       | (a) | V 119 | (a) | V 120 | (a) |
| 6             | -2.376589               | -2.341773 | -0.026833 | V 121                                       | (a) | V 122 | (a) | V 123 | (a) |
| 6             | -3.271026               | -1.119937 | -0.138003 | V 124                                       | (a) | V 125 | (a) | V 126 | (a) |
| 6             | -2.975419               | -0.277600 | -1.334455 | V 127                                       | (a) | V 128 | (a) | V 129 | (a) |
| 6             | -2.797760               | 1.139608  | -1.234836 | V 130                                       | (a) | V 131 | (a) | V 132 | (a) |
| 6             | -2.759417               | 1.778229  | 0.010666  | V 133                                       | (a) | V 134 | (a) | V 135 | (a) |
| 6             | -1.805343               | 2.834118  | 0.246587  | V 136                                       | (a) | V 137 | (a) | V 138 | (a) |
| 6             | 0.018693                | 2.982019  | 1.906687  | V 139                                       | (a) | V 140 | (a) | V 141 | (a) |
| 6             | -1.313917               | 2.702176  | 1.610675  | V 142                                       | (a) | V 143 | (a) | V 144 | (a) |
| 6             | -1.968544               | 1.553364  | 2.217232  | V 145                                       | (a) | V 146 | (a) | V 147 | (a) |
| 6             | -2.856606               | 0.972718  | 1.234774  | V 148                                       | (a) | V 149 | (a) | V 150 | (a) |
| 6             | -3.030034               | -0.398240 | 1.176716  | V 151                                       | (a) | V 152 | (a) | V 153 | (a) |
| 6             | -1.262922               | 0.731133  | 3.101058  | V 154                                       | (a) | V 155 | (a) | V 156 | (a) |
| 6             | 0.128650                | 1.018210  | 3.405346  | V 157                                       | (a) | V 158 | (a) | V 159 | (a) |
| 6             | 0.757113                | 2.119024  | 2.817952  | V 160                                       | (a) | V 161 | (a) | V 162 | (a) |
| 6             | -2.272318               | -1.248670 | 2.054304  | V 163                                       | (a) | V 164 | (a) | V 165 | (a) |
| 6             | -1.418999               | -0.704401 | 3.020571  | V 166                                       | (a) | V 167 | (a) | V 168 | (a) |
| 6             | -0.123093               | -1.314655 | 3.272561  | V 169                                       | (a) | V 170 | (a) | V 171 | (a) |
| 6             | 0.834435                | -0.248846 | 3.513042  | V 172                                       | (a) | V 173 | (a) | V 174 | (a) |
| 6             | 0.262838                | -2.455834 | 2.567125  | V 175                                       | (a) | V 176 | (a) | V 177 | (a) |
| 6             | -0.630270               | -3.034701 | 1.575114  | V 178                                       | (a) | V 179 | (a) | V 180 | (a) |
| 6             | -1.870168               | -2.439988 | 1.316735  | V 181                                       | (a) | V 182 | (a) | V 183 | (a) |
| 9             | -4.720022               | -1.569841 | -0.204096 |                                             |     |       |     |       |     |
| 3             | -5.961728               | -0.186218 | -0.022523 |                                             |     |       |     |       |     |
| 9             | -5.820128               | 1.405216  | 0.188886  |                                             |     |       |     |       |     |

The atomic coordinates for the C60AlCl4 equilibrium structure and the corresponding vibrational frequencies calculated using the B3LYP/6-31+G(d) method

| Atomic Number | Coordinates (Angstroms) |           |           | Vibrational frequencies [cm <sup>-1</sup> ] |     |           |       |     |           |       |     |           |      |     |          |
|---------------|-------------------------|-----------|-----------|---------------------------------------------|-----|-----------|-------|-----|-----------|-------|-----|-----------|------|-----|----------|
|               | x                       | y         | z         | V 1                                         | (a) | 11.0883   | V 2   | (a) | 13.8784   | V 3   | (a) | 18.6711   | V 4  | (a) | 30.8092  |
| 6             | -1.839003               | -3.484161 | -0.542594 | V 7                                         | (a) | 113.8529  | V 8   | (a) | 119.0436  | V 9   | (a) | 166.7288  | V 10 | (a) | 168.2727 |
| 6             | -0.442376               | -3.330131 | -0.913322 | V 13                                        | (a) | 261.3773  | V 14  | (a) | 263.2603  | V 15  | (a) | 264.0493  | V 16 | (a) | 265.4336 |
| 6             | 0.513405                | -3.055418 | 0.063554  | V 19                                        | (a) | 341.3728  | V 20  | (a) | 345.5442  | V 21  | (a) | 350.355   | V 17 | (a) | 329.5389 |
| 6             | 0.112837                | -2.921204 | 1.454574  | V 22                                        | (a) | 353.3033  | V 23  | (a) | 354.5414  | V 24  | (a) | 355.8449  | V 18 | (a) | 339.597  |
| 6             | -1.227367               | -3.066574 | 1.811027  | V 25                                        | (a) | 398.8257  | V 26  | (a) | 402.5348  | V 27  | (a) | 404.4402  | V 19 | (a) | 341.3728 |
| 6             | -2.224059               | -3.355092 | 0.793361  | V 28                                        | (a) | 407.1322  | V 29  | (a) | 408.105   | V 30  | (a) | 409.4691  | V 20 | (a) | 345.5442 |
| 6             | -2.65037                | -2.889595 | -1.593222 | V 31                                        | (a) | 426.8022  | V 32  | (a) | 430.1685  | V 33  | (a) | 432.4229  | V 21 | (a) | 350.355  |
| 6             | -1.753229               | -2.366732 | -2.612211 | V 34                                        | (a) | 436.0947  | V 35  | (a) | 441.4168  | V 36  | (a) | 479.1232  | V 22 | (a) | 353.3033 |
| 6             | -0.392268               | -2.635464 | -2.192672 | V 37                                        | (a) | 481.6608  | V 38  | (a) | 486.8333  | V 39  | (a) | 489.6481  | V 23 | (a) | 354.5414 |
| 6             | 0.613974                | -1.695906 | -2.443271 | V 40                                        | (a) | 490.3795  | V 41  | (a) | 496.0467  | V 42  | (a) | 521.5724  | V 24 | (a) | 354.5414 |
| 6             | 1.553491                | -2.073036 | -0.196601 | V 43                                        | (a) | 531.3673  | V 44  | (a) | 535.0232  | V 45  | (a) | 537.2987  | V 25 | (a) | 398.8257 |
| 6             | 0.90782                 | -1.855333 | 2.044677  | V 46                                        | (a) | 538.8443  | V 47  | (a) | 539.4155  | V 48  | (a) | 540.0477  | V 26 | (a) | 402.5348 |
| 6             | 0.330365                | -0.98023  | 2.970523  | V 49                                        | (a) | 541.1056  | V 50  | (a) | 543.4505  | V 51  | (a) | 564.1994  | V 27 | (a) | 402.5348 |
| 6             | -1.055103               | -1.135477 | 3.350627  | V 52                                        | (a) | 565.1249  | V 53  | (a) | 566.4993  | V 54  | (a) | 572.4229  | V 28 | (a) | 407.1322 |
| 6             | -1.824097               | -2.154823 | 2.776929  | V 55                                        | (a) | 573.8061  | V 56  | (a) | 575.3133  | V 57  | (a) | 575.8631  | V 29 | (a) | 408.105  |
| 6             | -3.186447               | -1.886331 | 2.360628  | V 58                                        | (a) | 576.5245  | V 59  | (a) | 577.2714  | V 60  | (a) | 579.7997  | V 30 | (a) | 409.4691 |
| 6             | -3.435658               | -2.625797 | 1.132994  | V 61                                        | (a) | 585.8452  | V 62  | (a) | 587.8176  | V 63  | (a) | 589.2629  | V 31 | (a) | 426.8022 |
| 6             | -4.214331               | -2.057609 | 0.124968  | V 64                                        | (a) | 676.2998  | V 65  | (a) | 676.7227  | V 66  | (a) | 677.3426  | V 32 | (a) | 430.1685 |
| 6             | -3.813746               | -2.192323 | -1.267093 | V 67                                        | (a) | 677.5707  | V 68  | (a) | 678.9282  | V 69  | (a) | 705.8421  | V 33 | (a) | 432.4229 |
| 6             | -2.058202               | -1.168296 | -3.266039 | V 70                                        | (a) | 706.9707  | V 71  | (a) | 709.9104  | V 72  | (a) | 716.1806  | V 34 | (a) | 436.0947 |
| 6             | -3.266504               | -0.445758 | -2.925645 | V 73                                        | (a) | 717.5083  | V 74  | (a) | 721.7588  | V 75  | (a) | 724.4499  | V 35 | (a) | 441.4168 |
| 6             | -4.128623               | -0.946084 | -1.946564 | V 76                                        | (a) | 725.5439  | V 77  | (a) | 736.9515  | V 78  | (a) | 739.0125  | V 36 | (a) | 479.1232 |
| 6             | -4.717749               | -0.04365  | -0.975207 | V 79                                        | (a) | 739.3195  | V 80  | (a) | 740.3274  | V 81  | (a) | 741.5107  | V 37 | (a) | 481.6608 |
| 6             | -4.776459               | -0.728515 | 0.302717  | V 82                                        | (a) | 744.3017  | V 83  | (a) | 745.7929  | V 84  | (a) | 746.1428  | V 38 | (a) | 486.8333 |
| 6             | -4.536971               | -0.019625 | 1.482265  | V 85                                        | (a) | 747.1256  | V 86  | (a) | 748.4049  | V 87  | (a) | 751.0251  | V 39 | (a) | 489.6481 |
| 6             | -3.72814                | -0.60804  | 2.53001   | V 88                                        | (a) | 752.8779  | V 89  | (a) | 755.2743  | V 90  | (a) | 756.201   | V 40 | (a) | 490.3795 |
| 6             | -2.93048                | 0.451965  | 3.131048  | V 91                                        | (a) | 759.7204  | V 92  | (a) | 763.416   | V 93  | (a) | 764.6798  | V 41 | (a) | 496.0467 |
| 6             | -1.622143               | 0.194184  | 3.53      | V 94                                        | (a) | 766.2713  | V 95  | (a) | 767.5403  | V 96  | (a) | 771.4401  | V 42 | (a) | 496.0467 |
| 6             | 1.78161                 | -1.334987 | 1.019809  | V 97                                        | (a) | 775.347   | V 98  | (a) | 782.2168  | V 99  | (a) | 787.3605  | V 43 | (a) | 531.3673 |
| 6             | 0.012512                | 2.895042  | 1.596745  | V 100                                       | (a) | 788.6345  | V 101 | (a) | 789.6554  | V 102 | (a) | 806.0366  | V 44 | (a) | 535.0232 |
| 6             | 1.174704                | 2.196717  | 1.269133  | V 103                                       | (a) | 806.4497  | V 104 | (a) | 808.2923  | V 105 | (a) | 840.3745  | V 45 | (a) | 537.2987 |
| 6             | 1.574682                | 2.06111   | -0.124605 | V 106                                       | (a) | 841.0596  | V 107 | (a) | 841.3977  | V 108 | (a) | 967.3535  | V 46 | (a) | 538.8443 |
| 6             | 0.799204                | 2.631086  | -1.131624 | V 109                                       | (a) | 972.2884  | V 110 | (a) | 975.7954  | V 111 | (a) | 977.5505  | V 47 | (a) | 539.4155 |
| 6             | -0.416117               | 3.354051  | -0.79078  | V 112                                       | (a) | 981.9093  | V 113 | (a) | 982.1696  | V 114 | (a) | 983.0684  | V 48 | (a) | 539.4155 |
| 6             | -2.196634               | 3.326014  | 0.915899  | V 115                                       | (a) | 984.4289  | V 116 | (a) | 1078.8564 | V 117 | (a) | 1086.6732 | V 49 | (a) | 541.1056 |
| 6             | -2.245615               | 2.636459  | 2.196423  | V 118                                       | (a) | 1102.9983 | V 119 | (a) | 1104.5813 | V 120 | (a) | 1121.2708 | V 50 | (a) | 543.4505 |
| 6             | -0.882133               | 2.369854  | 2.614638  | V 121                                       | (a) | 1123.2206 | V 122 | (a) | 1125.684  | V 123 | (a) | 1125.8948 | V 51 | (a) | 564.1994 |
| 6             | -0.574563               | 1.171843  | 3.267536  | V 124                                       | (a) | 1129.7478 | V 125 | (a) | 1192.9201 | V 126 | (a) | 1196.5517 | V 52 | (a) | 565.1249 |
| 6             | 0.632159                | 0.452236  | 2.922515  | V 127                                       | (a) | 1204.0851 | V 128 | (a) | 1206.7508 | V 129 | (a) | 1217.187  | V 53 | (a) | 566.4993 |
| 6             | 1.490924                | 0.954417  | 1.947699  | V 130                                       | (a) | 1221.7049 | V 131 | (a) | 1229.2197 | V 132 | (a) | 1231.0082 | V 54 | (a) | 566.4993 |
| 6             | 2.136947                | 0.736389  | -0.30278  | V 133                                       | (a) | 1238.6032 | V 134 | (a) | 1241.2599 | V 135 | (a) | 1242.7694 | V 55 | (a) | 573.8061 |
| 6             | 1.895134                | 0.026849  | -1.476435 | V 136                                       | (a) | 1257.3525 | V 137 | (a) | 1267.6103 | V 138 | (a) | 1272.0443 | V 56 | (a) | 575.3133 |
| 6             | 1.094471                | 0.611843  | -2.525018 | V 139                                       | (a) | 1277.5573 | V 140 | (a) | 1282.8407 | V 141 | (a) | 1296.4422 | V 57 | (a) | 575.8631 |
| 6             | 0.551204                | 1.890233  | -2.357379 | V 142                                       | (a) | 1303.0888 | V 143 | (a) | 1307.3059 | V 144 | (a) | 1322.2743 | V 58 | (a) | 576.5245 |
| 6             | -0.811178               | 2.156041  | -2.77594  | V 145                                       | (a) | 1327.7632 | V 146 | (a) | 1330.1391 | V 147 | (a) | 1333.4234 | V 59 | (a) | 585.8452 |
| 6             | -1.411204               | 3.062659  | -1.808173 | V 148                                       | (a) | 1333.6329 | V 149 | (a) | 1334.5289 | V 150 | (a) | 1336.5306 | V 60 | (a) | 576.5245 |
| 6             | -2.75321                | 2.914613  | -1.452558 | V 151                                       | (a) | 1337.5959 | V 152 | (a) | 1343.6978 | V 153 | (a) | 1357.1858 | V 61 | (a) | 585.8452 |
| 6             | -3.153759               | 3.048531  | -0.062034 | V 154                                       | (a) | 1368.504  | V 155 | (a) | 1368.805  | V 156 | (a) | 1370.3307 | V 62 | (a) | 587.8176 |
| 6             | -3.250056               | 1.697091  | 2.448071  | V 157                                       | (a) | 1371.9383 | V 158 | (a) | 1375.1271 | V 159 | (a) | 1376.4485 | V 63 | (a) | 587.8176 |
| 6             | -4.239475               | 1.406517  | 1.430466  | V 160                                       | (a) | 1382.8243 | V 161 | (a) | 1433.6928 | V 162 | (a) | 1435.4345 | V 64 | (a) | 676.2998 |
| 6             | -4.194369               | 2.068275  | 0.199956  | V 163                                       | (a) | 1446.1622 | V 164 | (a) | 1450.4903 | V 165 | (a) | 1451.9376 | V 65 | (a) | 676.7227 |
| 6             | -4.43335                | 1.329219  | -1.025542 | V 166                                       | (a) | 1453.453  | V 167 | (a) | 1458.0214 | V 168 | (a) | 1458.6405 | V 66 | (a) | 677.5707 |
| 6             | -3.546814               | 1.851619  | -2.046867 | V 169                                       | (a) | 1464.1524 | V 170 | (a) | 1465.183  | V 171 | (a) | 1466.3221 | V 67 | (a) | 677.5707 |
| 6             | -2.967637               | 0.980767  | -2.97578  | V 172                                       | (a) | 1505.0239 | V 173 | (a) | 1513.5754 | V 174 | (a) | 1523.7089 | V 68 | (a) | 678.9282 |
| 6             | -1.578384               | 1.13703   | -3.35097  | V 175                                       | (a) | 1529.5363 | V 176 | (a) | 1535.4118 | V 177 | (a) | 1550.3996 | V 69 | (a) | 678.9282 |
| 6             | -1.010451               | -0.191886 | -3.531109 | V 178                                       | (a) | 1556.4404 | V 179 | (a) | 1564.3062 | V 180 | (a) | 1573.1524 | V 70 | (a) | 706.9707 |
| 6             | 0.294981                | -0.449091 | -3.125492 | V 181                                       | (a) | 1585.3799 | V 182 | (a) | 1596.0619 | V 183 | (a) | 1597.699  | V 71 | (a) | 709.9104 |
| 6             | 2.089213                | 0.052652  | 0.974522  | V 184                                       | (a) | 1598.3481 | V 185 | (a) | 1601.5394 | V 186 | (a) | 1602.6555 | V 72 | (a) | 716.1806 |
| 6             | 1.595647                | -1.40528  | -1.424793 | V 187                                       | (a) | 1605.4936 | V 188 | (a) | 1609.9165 | V 189 | (a) | 1612.6726 | V 73 | (a) | 717.5083 |
| 6             | -0.801181               | 3.485383  | 0.545238  |                                             |     |           |       |     |           |       |     |           | V 74 | (a) | 721.7588 |
| 13            | 5.923291                | 0.012632  | -0.057464 |                                             |     |           |       |     |           |       |     |           | V 75 | (a) | 724.4499 |
| 17            | 5.155251                | -1.444285 | -1.46826  |                                             |     |           |       |     |           |       |     |           | V 76 | (a) | 725.5439 |
| 17            | 8.000993                | -0.261082 | 0.361458  |                                             |     |           |       |     |           |       |     |           | V 77 | (a) | 736.9515 |
| 17            | 4.820195                | -0.32805  | 1.847897  |                                             |     |           |       |     |           |       |     |           | V 78 | (a) | 739.0125 |
| 17            | 5.423695                | 2.006731  | -0.713467 |                                             |     |           |       |     |           |       |     |           | V 79 | (a) | 739.3195 |

The atomic coordinates for the C60MgCl3 equilibrium structure and the corresponding vibrational frequencies calculated using the B3LYP/6-31+G(d) method

| Coordinates (Angstroms) |           |           |           | Vibrational frequencies [cm <sup>-1</sup> ] |                         |                         |                         |                         |                         |          |  |
|-------------------------|-----------|-----------|-----------|---------------------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|----------|--|
| Atomic Number           | x         | y         | z         | V 1 (a <sup>+</sup> )                       | 8.3008                  | V 2 (a <sup>+</sup> )   | 12.0114                 | V 3 (a <sup>+</sup> )   | 23.2378                 |          |  |
| 6                       | -3.256946 | -1.316442 | 1.423186  | V 4 (a <sup>+</sup> )                       | 40.602                  | V 5 (a <sup>+</sup> )   | 47.2765                 | V 6 (a <sup>+</sup> )   | 56.5787                 |          |  |
|                         | -2.401588 | -1.416905 | 2.597932  | V 7 (a <sup>+</sup> )                       | 110.0629                | V 8 (a <sup>+</sup> )   | 114.0574                | V 9 (a <sup>+</sup> )   | 145.0466                |          |  |
|                         | -1.667724 | -0.307612 | 3.029342  | V 10 (a <sup>+</sup> )                      | 242.5858                | V 11 (a <sup>+</sup> )  | 255.5183                | V 12 (a <sup>+</sup> )  | 260.0772                |          |  |
|                         | -1.748943 | 0.939574  | 2.297976  | V 13 (a <sup>+</sup> )                      | 261.9818                | V 14 (a <sup>+</sup> )  | 264.2795                | V 15 (a <sup>+</sup> )  | 266.5929                |          |  |
|                         | -2.572948 | 1.039891  | 1.169728  | V 16 (a <sup>+</sup> )                      | 340.9832                | V 17 (a <sup>+</sup> )  | 341.4098                | V 18 (a <sup>+</sup> )  | 344.2198                |          |  |
|                         | -3.343695 | -0.111646 | 0.725958  | V 19 (a <sup>+</sup> )                      | 350.1223                | V 20 (a <sup>+</sup> )  | 352.0273                | V 21 (a <sup>+</sup> )  | 355.9894                |          |  |
|                         | -3.170085 | -2.571642 | 0.698652  | V 22 (a <sup>+</sup> )                      | 356.346                 | V 23 (a <sup>+</sup> )  | 366.0611                | V 24 (a <sup>+</sup> )  | 401.3018                |          |  |
|                         | -2.266748 | -3.449532 | 1.426312  | V 25 (a <sup>+</sup> )                      | 404.3271                | V 26 (a <sup>+</sup> )  | 404.5219                | V 27 (a <sup>+</sup> )  | 407.7723                |          |  |
|                         | -1.795061 | -2.734845 | 2.601826  | V 28 (a <sup>+</sup> )                      | 407.776                 | V 29 (a <sup>+</sup> )  | 428.518                 | V 30 (a <sup>+</sup> )  | 432.253                 |          |  |
|                         | -0.473449 | -2.890211 | 3.030603  | V 31 (a <sup>+</sup> )                      | 433.721                 | V 32 (a <sup>+</sup> )  | 435.7412                | V 33 (a <sup>+</sup> )  | 439.9938                |          |  |
|                         | -0.294224 | -0.471535 | 3.479530  | V 34 (a <sup>+</sup> )                      | 481.4154                | V 35 (a <sup>+</sup> )  | 484.8397                | V 36 (a <sup>+</sup> )  | 485.4991                |          |  |
|                         | -0.426043 | 1.558973  | 2.302590  | V 37 (a <sup>+</sup> )                      | 486.4288                | V 38 (a <sup>+</sup> )  | 490.562                 | V 39 (a <sup>+</sup> )  | 495.7117                |          |  |
|                         | 0.027667  | 2.244134  | 1.178461  | V 40 (a <sup>+</sup> )                      | 532.8768                | V 41 (a <sup>+</sup> )  | 534.507                 | V 42 (a <sup>+</sup> )  | 535.5841                |          |  |
|                         | -0.826156 | 2.369152  | 0.000000  | V 43 (a <sup>+</sup> )                      | 538.7163                | V 44 (a <sup>+</sup> )  | 540.5001                | V 45 (a <sup>+</sup> )  | 540.9109                |          |  |
|                         | -2.100424 | 1.736567  | 0.000000  | V 46 (a <sup>+</sup> )                      | 541.1545                | V 47 (a <sup>+</sup> )  | 544.3627                | V 48 (a <sup>+</sup> )  | 564.1769                |          |  |
|                         | -2.572948 | 1.039891  | -1.169728 | V 49 (a <sup>+</sup> )                      | 566.1472                | V 50 (a <sup>+</sup> )  | 566.4245                | V 51 (a <sup>+</sup> )  | 572.6794                |          |  |
|                         | -3.343695 | -0.111646 | -0.725958 | V 52 (a <sup>+</sup> )                      | 573.3776                | V 53 (a <sup>+</sup> )  | 575.7592                | V 54 (a <sup>+</sup> )  | 575.8943                |          |  |
|                         | 6         | -3.256946 | -1.316442 | -1.423186                                   | V 55 (a <sup>+</sup> )  | 577.0296                | V 56 (a <sup>+</sup> )  | 577.5829                | V 57 (a <sup>+</sup> )  | 579.6637 |  |
| -3.170085               |           | -2.571642 | -0.698652 | V 58 (a <sup>+</sup> )                      | 585.9216                | V 59 (a <sup>+</sup> )  | 587.7007                | V 60 (a <sup>+</sup> )  | 588.7771                |          |  |
| -1.399130               |           | -4.289303 | 0.727651  | V 61 (a <sup>+</sup> )                      | 676.8917                | V 62 (a <sup>+</sup> )  | 677.3573                | V 63 (a <sup>+</sup> )  | 677.4698                |          |  |
| -1.399130               |           | -4.289303 | -0.727651 | V 64 (a <sup>+</sup> )                      | 678.1067                | V 65 (a <sup>+</sup> )  | 678.8495                | V 66 (a <sup>+</sup> )  | 709.7901                |          |  |
| -2.266748               |           | -3.449532 | -1.426312 | V 67 (a <sup>+</sup> )                      | 709.9243                | V 68 (a <sup>+</sup> )  | 714.4062                | V 69 (a <sup>+</sup> )  | 714.5298                |          |  |
| -1.795061               |           | -2.734845 | -2.601826 | V 70 (a <sup>+</sup> )                      | 719.5252                | V 71 (a <sup>+</sup> )  | 723.6892                | V 72 (a <sup>+</sup> )  | 723.8559                |          |  |
| -2.401588               |           | -1.416905 | -2.597932 | V 73 (a <sup>+</sup> )                      | 725.8338                | V 74 (a <sup>+</sup> )  | 737.7741                | V 75 (a <sup>+</sup> )  | 739.3672                |          |  |
| -1.667724               |           | -0.307612 | -3.029342 | V 76 (a <sup>+</sup> )                      | 739.8348                | V 77 (a <sup>+</sup> )  | 741.7082                | V 78 (a <sup>+</sup> )  | 742.5777                |          |  |
| -1.748943               |           | 0.939574  | -2.297976 | V 79 (a <sup>+</sup> )                      | 744.6999                | V 80 (a <sup>+</sup> )  | 746.4926                | V 81 (a <sup>+</sup> )  | 748.0566                |          |  |
| -0.426043               |           | 1.558973  | -2.302590 | V 82 (a <sup>+</sup> )                      | 749.273                 | V 83 (a <sup>+</sup> )  | 751.0558                | V 84 (a <sup>+</sup> )  | 751.5388                |          |  |
| 0.027667                |           | 2.244134  | -1.178461 | V 85 (a <sup>+</sup> )                      | 753.3879                | V 86 (a <sup>+</sup> )  | 757.1141                | V 87 (a <sup>+</sup> )  | 759.6746                |          |  |
| 0.469737                |           | 0.685141  | 3.031065  | V 88 (a <sup>+</sup> )                      | 762.1452                | V 89 (a <sup>+</sup> )  | 762.268                 | V 90 (a <sup>+</sup> )  | 765.9279                |          |  |
| 3.160327                |           | 0.359478  | -0.699193 | V 91 (a <sup>+</sup> )                      | 768.43                  | V 92 (a <sup>+</sup> )  | 770.817                 | V 93 (a <sup>+</sup> )  | 772.3853                |          |  |
| 3.160327                |           | 0.359478  | 0.699193  | V 94 (a <sup>+</sup> )                      | 777.8581                | V 95 (a <sup>+</sup> )  | 778.4299                | V 96 (a <sup>+</sup> )  | 786.3889                |          |  |
| 3.247231                |           | -0.895183 | 1.424158  | V 97 (a <sup>+</sup> )                      | 787.2093                | V 98 (a <sup>+</sup> )  | 789.7006                | V 99 (a <sup>+</sup> )  | 806.2032                |          |  |
| 6                       |           | 3.331020  | -2.102666 | 0.726539                                    | V 100 (a <sup>+</sup> ) | 806.5657                | V 101 (a <sup>+</sup> ) | 807.406                 | V 102 (a <sup>+</sup> ) | 840.5637 |  |
| 6                       |           | 3.331020  | -2.102666 | -0.726539                                   | V 103 (a <sup>+</sup> ) | 841.4492                | V 104 (a <sup>+</sup> ) | 841.5036                | V 105 (a <sup>+</sup> ) | 967.4695 |  |
| 6                       |           | 2.397455  | -0.792610 | -2.599997                                   | V 106 (a <sup>+</sup> ) | 973.7592                | V 107 (a <sup>+</sup> ) | 975.4141                | V 108 (a <sup>+</sup> ) | 977.5056 |  |
| 6                       | 1.790790  | 0.527015  | -2.601553 | V 109 (a <sup>+</sup> )                     | 981.7441                | V 110 (a <sup>+</sup> ) | 981.8332                | V 111 (a <sup>+</sup> ) | 983.2952                |          |  |
| 6                       | 2.261910  | 1.239572  | -1.428031 | V 112 (a <sup>+</sup> )                     | 983.7712                | V 113 (a <sup>+</sup> ) | 1083.6818               | V 114 (a <sup>+</sup> ) | 1097.3939               |          |  |
| 6                       | 1.392071  | 2.077105  | -0.729090 | V 115 (a <sup>+</sup> )                     | 1101.6288               | V 116 (a <sup>+</sup> ) | 1102.0873               | V 117 (a <sup>+</sup> ) | 1120.7568               |          |  |
| 6                       | 1.392071  | 2.077105  | 0.729090  | V 118 (a <sup>+</sup> )                     | 1124.5038               | V 119 (a <sup>+</sup> ) | 1125.661                | V 120 (a <sup>+</sup> ) | 1126.1552               |          |  |
| 6                       | 2.261910  | 1.239572  | 1.428031  | V 121 (a <sup>+</sup> )                     | 1127.7783               | V 122 (a <sup>+</sup> ) | 1195.6673               | V 123 (a <sup>+</sup> ) | 1199.1776               |          |  |
| 6                       | 2.397455  | -0.792610 | 2.599997  | V 124 (a <sup>+</sup> )                     | 1208.103                | V 125 (a <sup>+</sup> ) | 1208.4086               | V 126 (a <sup>+</sup> ) | 1214.0741               |          |  |
| 6                       | 1.664056  | -1.900988 | 3.031822  | V 127 (a <sup>+</sup> )                     | 1214.158                | V 128 (a <sup>+</sup> ) | 1233.2885               | V 129 (a <sup>+</sup> ) | 1234.6675               |          |  |
| 6                       | 1.747600  | -3.152306 | 2.304100  | V 130 (a <sup>+</sup> )                     | 1241.4313               | V 131 (a <sup>+</sup> ) | 1242.0345               | V 132 (a <sup>+</sup> ) | 1243.1377               |          |  |
| 6                       | 2.565854  | -3.253038 | 1.174372  | V 133 (a <sup>+</sup> )                     | 1263.5403               | V 134 (a <sup>+</sup> ) | 1265.0104               | V 135 (a <sup>+</sup> ) | 1274.0664               |          |  |
| 6                       | 2.092961  | -3.963705 | 0.000000  | V 136 (a <sup>+</sup> )                     | 1278.997                | V 137 (a <sup>+</sup> ) | 1281.3285               | V 138 (a <sup>+</sup> ) | 1299.1396               |          |  |
| 6                       | 2.565854  | -3.253038 | -1.174372 | V 139 (a <sup>+</sup> )                     | 1301.483                | V 140 (a <sup>+</sup> ) | 1305.8094               | V 141 (a <sup>+</sup> ) | 1323.3866               |          |  |
| 6                       | 1.747600  | -3.152306 | -2.304100 | V 142 (a <sup>+</sup> )                     | 1327.6049               | V 143 (a <sup>+</sup> ) | 1330.8949               | V 144 (a <sup>+</sup> ) | 1332.5371               |          |  |
| 6                       | 1.664056  | -1.900988 | -3.031822 | V 145 (a <sup>+</sup> )                     | 1333.7838               | V 146 (a <sup>+</sup> ) | 1334.1285               | V 147 (a <sup>+</sup> ) | 1337.5523               |          |  |
| 6                       | 0.469737  | 0.685141  | -3.031065 | V 148 (a <sup>+</sup> )                     | 1338.5823               | V 149 (a <sup>+</sup> ) | 1353.8846               | V 150 (a <sup>+</sup> ) | 1363.0121               |          |  |
| 6                       | -0.294224 | -0.471535 | -3.479530 | V 151 (a <sup>+</sup> )                     | 1367.538                | V 152 (a <sup>+</sup> ) | 1368.1962               | V 153 (a <sup>+</sup> ) | 1369.377                |          |  |
| 6                       | 0.290310  | -1.735532 | -3.481887 | V 154 (a <sup>+</sup> )                     | 1371.9422               | V 155 (a <sup>+</sup> ) | 1375.0285               | V 156 (a <sup>+</sup> ) | 1376.0368               |          |  |
| 6                       | -0.473449 | -2.890211 | -3.030603 | V 157 (a <sup>+</sup> )                     | 1398.4247               | V 158 (a <sup>+</sup> ) | 1424.4646               | V 159 (a <sup>+</sup> ) | 1430.0214               |          |  |
| 6                       | 0.426455  | -3.766078 | -2.304850 | V 160 (a <sup>+</sup> )                     | 1448.6543               | V 161 (a <sup>+</sup> ) | 1450.5855               | V 162 (a <sup>+</sup> ) | 1452.6414               |          |  |
| 6                       | -0.025747 | -4.452385 | -1.176160 | V 163 (a <sup>+</sup> )                     | 1454.5208               | V 164 (a <sup>+</sup> ) | 1457.1695               | V 165 (a <sup>+</sup> ) | 1459.3357               |          |  |
| 6                       | 0.821293  | -4.548353 | 0.000000  | V 166 (a <sup>+</sup> )                     | 1461.9917               | V 167 (a <sup>+</sup> ) | 1464.5612               | V 168 (a <sup>+</sup> ) | 1465.148                |          |  |
| 6                       | -0.025747 | -4.452385 | 1.176160  | V 169 (a <sup>+</sup> )                     | 1502.8609               | V 170 (a <sup>+</sup> ) | 1520.5975               | V 171 (a <sup>+</sup> ) | 1521.8007               |          |  |
| 6                       | 0.426455  | -3.766078 | 2.304850  | V 172 (a <sup>+</sup> )                     | 1532.1906               | V 173 (a <sup>+</sup> ) | 1536.5874               | V 174 (a <sup>+</sup> ) | 1552.3839               |          |  |
| 6                       | 1.790790  | 0.527015  | 2.601553  | V 175 (a <sup>+</sup> )                     | 1557.2824               | V 176 (a <sup>+</sup> ) | 1564.4068               | V 177 (a <sup>+</sup> ) | 1579.1726               |          |  |
| 6                       | 0.290310  | -1.735532 | 3.481887  | V 178 (a <sup>+</sup> )                     | 1584.7849               | V 179 (a <sup>+</sup> ) | 1597.3738               | V 180 (a <sup>+</sup> ) | 1598.7636               |          |  |
| 6                       | 3.247231  | -0.895183 | -1.424158 | V 181 (a <sup>+</sup> )                     | 1600.2401               | V 182 (a <sup>+</sup> ) | 1601.4433               | V 183 (a <sup>+</sup> ) | 1602.9862               |          |  |
| 12                      | 0.121580  | 6.426952  | 0.000000  | V 184 (a <sup>+</sup> )                     | 1605.1158               | V 185 (a <sup>+</sup> ) | 1610.4198               | V 186 (a <sup>+</sup> ) | 1611.6282               |          |  |
| 17                      | -1.708948 | 4.926834  | 0.000000  |                                             |                         |                         |                         |                         |                         |          |  |
| 17                      | -0.434784 | 8.600767  | 0.000000  |                                             |                         |                         |                         |                         |                         |          |  |
| 17                      | 2.111565  | 5.330606  | 0.000000  |                                             |                         |                         |                         |                         |                         |          |  |



