

## Electronic supporting information for manuscript:

### Charge assisted halogen and pnictogen bonds: insights from the Cambridge Structural Database and DFT calculations

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#### Cartesian coordinates of all compounds and complexes:

##### 1a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | -1.792734 | -0.000207 | -0.000080 |
| 2  | 9  | -1.234495 | 0.247761  | -1.282037 |
| 3  | 9  | -3.147409 | 0.007430  | -0.007586 |
| 4  | 9  | -1.251550 | -1.240446 | 0.428163  |
| 5  | 9  | -1.242036 | 0.985854  | 0.860809  |
| 6  | 15 | 1.304596  | 0.000248  | -0.000271 |
| 7  | 9  | 0.964235  | 1.362676  | -0.467436 |
| 8  | 9  | 0.960383  | -1.085729 | -0.944859 |
| 9  | 9  | 0.957828  | -0.275360 | 1.411663  |
| 10 | 9  | 2.814680  | -0.002484 | 0.001778  |

##### 1b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -2.299637 |
| 2  | 9  | 0.000000  | 0.000000  | -3.670880 |
| 3  | 9  | 0.000000  | 1.320620  | -1.784755 |
| 4  | 9  | -1.143691 | -0.660310 | -1.784755 |
| 5  | 9  | 1.143691  | -0.660310 | -1.784755 |
| 6  | 15 | 0.000000  | 0.000000  | 1.790566  |
| 7  | 9  | -1.202899 | 0.694494  | 2.327613  |
| 8  | 9  | -0.000000 | -1.388989 | 2.327613  |
| 9  | 9  | 1.202899  | 0.694494  | 2.327613  |
| 10 | 9  | 0.000000  | 0.000000  | 0.335604  |

##### 2a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -2.443018 |
| 2  | 9  | -1.141403 | 0.658989  | -1.924749 |
| 3  | 9  | 0.000000  | 0.000000  | -3.810973 |
| 4  | 9  | 1.141403  | 0.658989  | -1.924749 |
| 5  | 9  | -0.000000 | -1.317978 | -1.924749 |
| 6  | 15 | 0.000000  | 0.000000  | 1.130850  |
| 7  | 17 | 0.000000  | 0.000000  | 3.109120  |
| 8  | 17 | 0.000000  | 1.847327  | 0.562045  |
| 9  | 17 | 1.599832  | -0.923663 | 0.562045  |
| 10 | 17 | -1.599832 | -0.923663 | 0.562045  |

##### 2b

|   |    |           |           |           |
|---|----|-----------|-----------|-----------|
| 1 | 5  | 0.000000  | 0.000000  | 3.260244  |
| 2 | 9  | 0.000000  | 0.000000  | 4.626541  |
| 3 | 9  | 1.138124  | 0.657096  | 2.730568  |
| 4 | 9  | -0.000000 | -1.314193 | 2.730568  |
| 5 | 9  | -1.138124 | 0.657096  | 2.730568  |
| 6 | 15 | 0.000000  | 0.000000  | -1.531883 |
| 7 | 17 | -0.000000 | 1.826671  | -2.254441 |
| 8 | 17 | 0.000000  | 0.000000  | 0.369959  |
| 9 | 17 | 1.581944  | -0.913336 | -2.254441 |

|           |    |    |           |           |           |
|-----------|----|----|-----------|-----------|-----------|
|           | 10 | 17 | -1.581944 | -0.913336 | -2.254441 |
| <b>3a</b> |    |    |           |           |           |
|           | 1  | 5  | 0.000000  | 0.000000  | -2.963566 |
|           | 2  | 9  | -1.142329 | 0.659524  | -2.449300 |
|           | 3  | 9  | 0.000000  | 0.000000  | -4.333026 |
|           | 4  | 9  | 1.142329  | 0.659524  | -2.449300 |
|           | 5  | 9  | -0.000000 | -1.319048 | -2.449300 |
|           | 6  | 15 | 0.000000  | 0.000000  | 0.709169  |
|           | 7  | 35 | 0.000000  | 2.021715  | 0.083092  |
|           | 8  | 35 | 1.750856  | -1.010857 | 0.083092  |
|           | 9  | 35 | 0.000000  | 0.000000  | 2.873828  |
|           | 10 | 35 | -1.750856 | -1.010857 | 0.083092  |
| <b>3b</b> |    |    |           |           |           |
|           | 1  | 5  | 0.000000  | 0.000000  | 4.052963  |
|           | 2  | 9  | 0.000000  | 0.000000  | 5.415398  |
|           | 3  | 9  | 0.000000  | -1.312109 | 3.515543  |
|           | 4  | 9  | -1.136320 | 0.656055  | 3.515543  |
|           | 5  | 9  | 1.136320  | 0.656055  | 3.515543  |
|           | 6  | 15 | 0.000000  | 0.000000  | -0.986507 |
|           | 7  | 35 | 0.000000  | 1.998874  | -1.788031 |
|           | 8  | 35 | -1.731076 | -0.999437 | -1.788031 |
|           | 9  | 35 | 0.000000  | 0.000000  | 1.103365  |
|           | 10 | 35 | 1.731076  | -0.999437 | -1.788031 |
| <b>4a</b> |    |    |           |           |           |
|           | 1  | 5  | 0.000000  | 0.000000  | -3.256826 |
|           | 2  | 9  | -1.142781 | 0.659785  | -2.744938 |
|           | 3  | 9  | 0.000000  | 0.000000  | -4.627003 |
|           | 4  | 9  | 1.142781  | 0.659785  | -2.744938 |
|           | 5  | 9  | -0.000000 | -1.319570 | -2.744938 |
|           | 6  | 15 | 0.000000  | 0.000000  | 0.503082  |
|           | 7  | 53 | 0.000000  | 0.000000  | 2.912607  |
|           | 8  | 53 | 0.000000  | 2.259347  | -0.187886 |
|           | 9  | 53 | 1.956652  | -1.129674 | -0.187886 |
|           | 10 | 53 | -1.956652 | -1.129674 | -0.187886 |
| <b>4b</b> |    |    |           |           |           |
|           | 1  | 5  | 0.000000  | 0.000000  | 4.635407  |
|           | 2  | 9  | 0.000000  | 0.000000  | 5.993752  |
|           | 3  | 9  | -1.133835 | 0.654620  | 4.088912  |
|           | 4  | 9  | 1.133835  | 0.654620  | 4.088912  |
|           | 5  | 9  | -0.000000 | -1.309240 | 4.088912  |
|           | 6  | 15 | 0.000000  | 0.000000  | -0.739381 |
|           | 7  | 53 | 0.000000  | 2.225597  | -1.644361 |
|           | 8  | 53 | 1.927423  | -1.112798 | -1.644361 |
|           | 9  | 53 | -1.927423 | -1.112798 | -1.644361 |
|           | 10 | 53 | 0.000000  | 0.000000  | 1.604202  |
| <b>5a</b> |    |    |           |           |           |
|           | 1  | 5  | 0.000000  | 0.000000  | -2.682667 |
|           | 2  | 9  | 1.133868  | 0.654639  | -2.133991 |
|           | 3  | 9  | 0.000000  | 0.000000  | -4.038188 |
|           | 4  | 9  | -0.000000 | -1.309278 | -2.133991 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 5  | 9  | -1.133868 | 0.654639  | -2.133991 |
| 6  | 15 | 0.000000  | 0.000000  | 0.425165  |
| 7  | 9  | 0.000000  | 1.437968  | 0.074833  |
| 8  | 9  | 1.245317  | -0.718984 | 0.074833  |
| 9  | 9  | -1.245317 | -0.718984 | 0.074833  |
| 10 | 9  | 0.000000  | 0.000000  | 1.932625  |
| 11 | 8  | 0.000000  | 0.000000  | 6.308244  |
| 12 | 6  | 0.000000  | 0.000000  | 5.186210  |

## 5b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.062626 |
| 2  | 9  | 0.000000  | 0.000000  | -4.435143 |
| 3  | 9  | 1.143850  | 0.660402  | -2.549649 |
| 4  | 9  | -1.143850 | 0.660402  | -2.549649 |
| 5  | 9  | -0.000000 | -1.320804 | -2.549649 |
| 6  | 15 | 0.000000  | 0.000000  | 1.040446  |
| 7  | 9  | 0.000000  | 1.396509  | 1.556024  |
| 8  | 9  | -1.209412 | -0.698254 | 1.556024  |
| 9  | 9  | 1.209412  | -0.698254 | 1.556024  |
| 10 | 9  | 0.000000  | 0.000000  | -0.416912 |
| 11 | 8  | 0.000000  | 0.000000  | 5.494084  |
| 12 | 6  | 0.000000  | 0.000000  | 4.375025  |

## 6a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -2.650684 |
| 2  | 9  | 1.134723  | 0.655133  | -2.105985 |
| 3  | 9  | 0.000000  | 0.000000  | -4.008313 |
| 4  | 9  | -0.000000 | -1.310266 | -2.105985 |
| 5  | 9  | -1.134723 | 0.655133  | -2.105985 |
| 6  | 15 | 0.000000  | 0.000000  | 0.484440  |
| 7  | 9  | -0.000000 | 1.434500  | 0.119284  |
| 8  | 9  | 1.242314  | -0.717250 | 0.119284  |
| 9  | 9  | -1.242314 | -0.717250 | 0.119284  |
| 10 | 9  | 0.000000  | 0.000000  | 1.986736  |
| 11 | 6  | 0.000000  | 0.000000  | 6.054812  |
| 12 | 1  | 0.000000  | 0.000000  | 7.124445  |
| 13 | 7  | 0.000000  | 0.000000  | 4.909800  |

## 6b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.015044 |
| 2  | 9  | 0.000000  | 0.000000  | -4.389760 |
| 3  | 9  | 1.144235  | 0.660624  | -2.505764 |
| 4  | 9  | -1.144235 | 0.660624  | -2.505764 |
| 5  | 9  | -0.000000 | -1.321249 | -2.505764 |
| 6  | 15 | 0.000000  | 0.000000  | 1.118602  |
| 7  | 9  | 0.000000  | 1.408527  | 1.598351  |
| 8  | 9  | -1.219820 | -0.704264 | 1.598351  |
| 9  | 9  | 1.219820  | -0.704264 | 1.598351  |
| 10 | 9  | 0.000000  | 0.000000  | -0.343166 |
| 11 | 6  | 0.000000  | 0.000000  | 5.165687  |
| 12 | 1  | 0.000000  | 0.000000  | 6.236804  |
| 13 | 7  | 0.000000  | 0.000000  | 4.023107  |

**7a**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -2.384874 |
| 2  | 9  | 1.134751  | 0.655149  | -1.840065 |
| 3  | 9  | 0.000000  | 0.000000  | -3.742348 |
| 4  | 9  | -0.000000 | -1.310298 | -1.840065 |
| 5  | 9  | -1.134751 | 0.655149  | -1.840065 |
| 6  | 15 | 0.000000  | 0.000000  | 0.753322  |
| 7  | 9  | -0.000000 | 1.433966  | 0.385370  |
| 8  | 9  | 1.241851  | -0.716983 | 0.385370  |
| 9  | 9  | -1.241851 | -0.716983 | 0.385370  |
| 10 | 9  | 0.000000  | 0.000000  | 2.254850  |
| 11 | 7  | 0.000000  | 0.000000  | 5.213404  |
| 12 | 1  | -0.811857 | -0.468726 | 5.598318  |
| 13 | 1  | 0.000000  | 0.937452  | 5.598318  |
| 14 | 1  | 0.811857  | -0.468726 | 5.598318  |

**7b**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -2.667841 |
| 2  | 9  | 0.000000  | 0.000000  | -4.050763 |
| 3  | 9  | 1.146079  | 0.661689  | -2.171702 |
| 4  | 9  | -1.146079 | 0.661689  | -2.171702 |
| 5  | 9  | -0.000000 | -1.323378 | -2.171702 |
| 6  | 15 | 0.000000  | 0.000000  | 1.575784  |
| 7  | 9  | 0.000000  | 1.518884  | 1.759209  |
| 8  | 9  | -1.315392 | -0.759442 | 1.759209  |
| 9  | 9  | 1.315392  | -0.759442 | 1.759209  |
| 10 | 9  | 0.000000  | 0.000000  | 0.081503  |
| 11 | 7  | 0.000000  | 0.000000  | 3.548105  |
| 12 | 1  | 0.825170  | 0.476412  | 3.908788  |
| 13 | 1  | -0.000000 | -0.952825 | 3.908788  |
| 14 | 1  | -0.825170 | 0.476412  | 3.908788  |

**8a**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.467540 |
| 2  | 9  | 1.137247  | 0.656590  | -2.938814 |
| 3  | 9  | 0.000000  | 0.000000  | -4.835270 |
| 4  | 9  | -0.000000 | -1.313180 | -2.938814 |
| 5  | 9  | -1.137247 | 0.656590  | -2.938814 |
| 6  | 15 | 0.000000  | 0.000000  | -0.217354 |
| 7  | 9  | 0.000000  | 1.421252  | -0.634780 |
| 8  | 9  | 1.230840  | -0.710626 | -0.634780 |
| 9  | 9  | -1.230840 | -0.710626 | -0.634780 |
| 10 | 9  | 0.000000  | 0.000000  | 1.268560  |
| 11 | 6  | 0.000000  | 0.000000  | 5.774339  |
| 12 | 7  | 0.000000  | 0.000000  | 6.943057  |
| 13 | 16 | 0.000000  | 0.000000  | 4.121125  |

**8b**

|   |   |          |          |           |
|---|---|----------|----------|-----------|
| 1 | 5 | 0.000000 | 0.000000 | -3.785431 |
|---|---|----------|----------|-----------|

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 2  | 9  | 0.000000  | 0.000000  | -5.171549 |
| 3  | 9  | 1.144958  | 0.661042  | -3.290469 |
| 4  | 9  | -1.144958 | 0.661042  | -3.290469 |
| 5  | 9  | -0.000000 | -1.322084 | -3.290469 |
| 6  | 15 | 0.000000  | 0.000000  | 0.466213  |
| 7  | 9  | 0.000000  | 1.421991  | 0.896034  |
| 8  | 9  | -1.231480 | -0.710995 | 0.896034  |
| 9  | 9  | 1.231480  | -0.710995 | 0.896034  |
| 10 | 9  | 0.000000  | 0.000000  | -1.009665 |
| 11 | 6  | 0.000000  | 0.000000  | 5.188123  |
| 12 | 7  | 0.000000  | 0.000000  | 6.353540  |
| 13 | 16 | 0.000000  | 0.000000  | 3.538194  |

### 9a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.481736 |
| 2  | 9  | 1.138646  | 0.657398  | -2.961459 |
| 3  | 9  | 0.000000  | 0.000000  | -4.854693 |
| 4  | 9  | -0.000000 | -1.314795 | -2.961459 |
| 5  | 9  | -1.138646 | 0.657398  | -2.961459 |
| 6  | 15 | 0.000000  | 0.000000  | -0.163536 |
| 7  | 9  | 0.000000  | 1.415729  | -0.614501 |
| 8  | 9  | 1.226057  | -0.707865 | -0.614501 |
| 9  | 9  | -1.226057 | -0.707865 | -0.614501 |
| 10 | 9  | 0.000000  | 0.000000  | 1.321422  |
| 11 | 35 | 0.000000  | 0.000000  | 4.234631  |

### 9b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.712856 |
| 2  | 9  | 0.000000  | 0.000000  | -5.115839 |
| 3  | 9  | 1.147658  | 0.662600  | -3.241617 |
| 4  | 9  | -1.147658 | 0.662600  | -3.241617 |
| 5  | 9  | -0.000000 | -1.325201 | -3.241617 |
| 6  | 15 | 0.000000  | 0.000000  | 0.968926  |
| 7  | 9  | 0.000000  | 1.544556  | 1.024295  |
| 8  | 9  | -1.337625 | -0.772278 | 1.024295  |
| 9  | 9  | 1.337625  | -0.772278 | 1.024295  |
| 10 | 9  | 0.000000  | 0.000000  | -0.571763 |
| 11 | 35 | 0.000000  | 0.000000  | 3.288186  |

### 10a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.165762 |
| 2  | 9  | -1.141579 | 0.659091  | -2.648481 |
| 3  | 9  | 0.000000  | 0.000000  | -4.534307 |
| 4  | 9  | 1.141579  | 0.659091  | -2.648481 |
| 5  | 9  | -0.000000 | -1.318182 | -2.648481 |
| 6  | 15 | 0.000000  | 0.000000  | 0.421244  |
| 7  | 17 | 0.000000  | 0.000000  | 2.397098  |
| 8  | 17 | 0.000000  | 1.846601  | -0.154214 |
| 9  | 17 | 1.599203  | -0.923300 | -0.154214 |
| 10 | 17 | -1.599203 | -0.923300 | -0.154214 |
| 11 | 8  | 0.000000  | 0.000000  | 6.833689  |
| 12 | 6  | 0.000000  | 0.000000  | 5.712106  |

**10b**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 3.882330  |
| 2  | 9  | 0.000000  | 0.000000  | 5.249354  |
| 3  | 9  | 1.138306  | 0.657201  | 3.353745  |
| 4  | 9  | -0.000000 | -1.314403 | 3.353745  |
| 5  | 9  | -1.138306 | 0.657201  | 3.353745  |
| 6  | 15 | 0.000000  | 0.000000  | -0.917776 |
| 7  | 17 | 0.000000  | 1.829284  | -1.630844 |
| 8  | 17 | 0.000000  | 0.000000  | 0.985360  |
| 9  | 17 | 1.584206  | -0.914642 | -1.630844 |
| 10 | 17 | -1.584206 | -0.914642 | -1.630844 |
| 11 | 8  | 0.000000  | 0.000000  | -5.981905 |
| 12 | 6  | 0.000000  | 0.000000  | -4.860521 |

**11a**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.145700 |
| 2  | 9  | -1.141906 | 0.659279  | -2.630872 |
| 3  | 9  | 0.000000  | 0.000000  | -4.516057 |
| 4  | 9  | 1.141906  | 0.659279  | -2.630872 |
| 5  | 9  | -0.000000 | -1.318559 | -2.630872 |
| 6  | 15 | 0.000000  | 0.000000  | 0.463851  |
| 7  | 17 | 0.000000  | 0.000000  | 2.432646  |
| 8  | 17 | 0.000000  | 1.844735  | -0.124253 |
| 9  | 17 | 1.597587  | -0.922367 | -0.124253 |
| 10 | 17 | -1.597587 | -0.922367 | -0.124253 |
| 11 | 6  | 0.000000  | 0.000000  | 6.597981  |
| 12 | 1  | 0.000000  | 0.000000  | 7.667713  |
| 13 | 7  | 0.000000  | 0.000000  | 5.453587  |

**11b**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 3.857449  |
| 2  | 9  | 0.000000  | 0.000000  | 5.226427  |
| 3  | 9  | 1.138842  | 0.657511  | 3.332099  |
| 4  | 9  | -0.000000 | -1.315021 | 3.332099  |
| 5  | 9  | -1.138842 | 0.657511  | 3.332099  |
| 6  | 15 | 0.000000  | 0.000000  | -0.966905 |
| 7  | 17 | 0.000000  | 1.832062  | -1.665849 |
| 8  | 17 | 0.000000  | 0.000000  | 0.939920  |
| 9  | 17 | 1.586612  | -0.916031 | -1.665849 |
| 10 | 17 | -1.586612 | -0.916031 | -1.665849 |
| 11 | 6  | 0.000000  | 0.000000  | -5.696515 |
| 12 | 1  | 0.000000  | 0.000000  | -6.766666 |
| 13 | 7  | 0.000000  | 0.000000  | -4.551820 |

**12a**

|   |   |           |          |           |
|---|---|-----------|----------|-----------|
| 1 | 5 | 0.000000  | 0.000000 | -2.916174 |
| 2 | 9 | -1.142021 | 0.659346 | -2.402019 |
| 3 | 9 | 0.000000  | 0.000000 | -4.286844 |
| 4 | 9 | 1.142021  | 0.659346 | -2.402019 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 5  | 9  | -0.000000 | -1.318692 | -2.402019 |
| 6  | 15 | 0.000000  | 0.000000  | 0.707009  |
| 7  | 17 | 0.000000  | 0.000000  | 2.682984  |
| 8  | 17 | 0.000000  | 1.844246  | 0.108889  |
| 9  | 17 | 1.597164  | -0.922123 | 0.108889  |
| 10 | 17 | -1.597164 | -0.922123 | 0.108889  |
| 11 | 7  | 0.000000  | 0.000000  | 5.512093  |
| 12 | 1  | -0.814841 | -0.470449 | 5.887703  |
| 13 | 1  | 0.000000  | 0.940897  | 5.887703  |
| 14 | 1  | 0.814841  | -0.470449 | 5.887703  |

## 12b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 3.656258  |
| 2  | 9  | 0.000000  | 0.000000  | 5.025223  |
| 3  | 9  | 1.138857  | 0.657519  | 3.130949  |
| 4  | 9  | -0.000000 | -1.315038 | 3.130949  |
| 5  | 9  | -1.138857 | 0.657519  | 3.130949  |
| 6  | 15 | 0.000000  | 0.000000  | -1.169872 |
| 7  | 17 | 0.000000  | 1.837737  | -1.854386 |
| 8  | 17 | 0.000000  | 0.000000  | 0.737890  |
| 9  | 17 | 1.591527  | -0.918868 | -1.854386 |
| 10 | 17 | -1.591527 | -0.918868 | -1.854386 |
| 11 | 7  | 0.000000  | 0.000000  | -4.729706 |
| 12 | 1  | 0.000000  | 0.936221  | -5.119449 |
| 13 | 1  | -0.810791 | -0.468110 | -5.119449 |
| 14 | 1  | 0.810791  | -0.468110 | -5.119449 |

## 13a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.861063 |
| 2  | 9  | -1.143318 | 0.660095  | -3.359973 |
| 3  | 9  | 0.000000  | 0.000000  | -5.241613 |
| 4  | 9  | 1.143318  | 0.660095  | -3.359973 |
| 5  | 9  | -0.000000 | -1.320190 | -3.359973 |
| 6  | 15 | 0.000000  | 0.000000  | -0.101912 |
| 7  | 17 | 0.000000  | 0.000000  | 1.840852  |
| 8  | 17 | 0.000000  | 1.835049  | -0.752310 |
| 9  | 17 | 1.589199  | -0.917524 | -0.752310 |
| 10 | 17 | -1.589199 | -0.917524 | -0.752310 |
| 11 | 6  | 0.000000  | 0.000000  | 6.347519  |
| 12 | 7  | 0.000000  | 0.000000  | 7.514862  |
| 13 | 16 | 0.000000  | 0.000000  | 4.694498  |

## 13b

|   |    |           |           |           |
|---|----|-----------|-----------|-----------|
| 1 | 5  | 0.000000  | 0.000000  | 4.536177  |
| 2 | 9  | 0.000000  | 0.000000  | 5.916249  |
| 3 | 9  | 1.140944  | 0.658724  | 4.027321  |
| 4 | 9  | -0.000000 | -1.317448 | 4.027321  |
| 5 | 9  | -1.140944 | 0.658724  | 4.027321  |
| 6 | 15 | 0.000000  | 0.000000  | -0.427333 |
| 7 | 17 | 0.000000  | 1.832280  | -1.097534 |
| 8 | 17 | 0.000000  | 0.000000  | 1.497140  |
| 9 | 17 | 1.586801  | -0.916140 | -1.097534 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 10 | 17 | -1.586801 | -0.916140 | -1.097534 |
| 11 | 6  | 0.000000  | 0.000000  | -5.724912 |
| 12 | 7  | 0.000000  | 0.000000  | -6.892158 |
| 13 | 16 | 0.000000  | 0.000000  | -4.071086 |

#### 14a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.941337 |
| 2  | 9  | -1.144938 | 0.661030  | -3.451839 |
| 3  | 9  | 0.000000  | 0.000000  | -5.330499 |
| 4  | 9  | 1.144938  | 0.661030  | -3.451839 |
| 5  | 9  | -0.000000 | -1.322060 | -3.451839 |
| 6  | 15 | 0.000000  | 0.000000  | -0.012690 |
| 7  | 17 | 0.000000  | 0.000000  | 2.050178  |
| 8  | 17 | 0.000000  | 1.836073  | -0.741674 |
| 9  | 17 | 1.590086  | -0.918036 | -0.741674 |
| 10 | 17 | -1.590086 | -0.918036 | -0.741674 |
| 11 | 35 | 0.000000  | 0.000000  | 4.686958  |

#### 14b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -4.342525 |
| 2  | 9  | 0.000000  | 0.000000  | -5.740141 |
| 3  | 9  | -1.145051 | 0.661095  | -3.860496 |
| 4  | 9  | -0.000000 | -1.322191 | -3.860496 |
| 5  | 9  | 1.145051  | 0.661095  | -3.860496 |
| 6  | 15 | 0.000000  | 0.000000  | 1.040304  |
| 7  | 17 | 0.000000  | 2.032418  | 1.136820  |
| 8  | 17 | 0.000000  | 0.000000  | -0.998475 |
| 9  | 17 | -1.760126 | -1.016209 | 1.136820  |
| 10 | 17 | 1.760126  | -1.016209 | 1.136820  |
| 11 | 35 | 0.000000  | 0.000000  | 3.457114  |

#### 15a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.425050 |
| 2  | 9  | -1.142451 | 0.659595  | -2.911757 |
| 3  | 9  | 0.000000  | 0.000000  | -4.795172 |
| 4  | 9  | 1.142451  | 0.659595  | -2.911757 |
| 5  | 9  | -0.000000 | -1.319189 | -2.911757 |
| 6  | 15 | 0.000000  | 0.000000  | 0.261475  |
| 7  | 35 | -0.000000 | 2.020622  | -0.373377 |
| 8  | 35 | 1.749910  | -1.010311 | -0.373377 |
| 9  | 35 | 0.000000  | 0.000000  | 2.424628  |
| 10 | 35 | -1.749910 | -1.010311 | -0.373377 |
| 11 | 8  | 0.000000  | 0.000000  | 6.860560  |
| 12 | 6  | 0.000000  | 0.000000  | 5.739218  |

#### 15b

|   |   |           |           |          |
|---|---|-----------|-----------|----------|
| 1 | 5 | 0.000000  | 0.000000  | 4.411502 |
| 2 | 9 | 0.000000  | 0.000000  | 5.775136 |
| 3 | 9 | 0.000000  | -1.312370 | 3.876047 |
| 4 | 9 | -1.136546 | 0.656185  | 3.876047 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 5  | 9  | 1.136546  | 0.656185  | 3.876047  |
| 6  | 15 | 0.000000  | 0.000000  | -0.632573 |
| 7  | 35 | 0.000000  | 2.000522  | -1.427942 |
| 8  | 35 | -1.732502 | -1.000261 | -1.427942 |
| 9  | 35 | 0.000000  | 0.000000  | 1.458385  |
| 10 | 35 | 1.732502  | -1.000261 | -1.427942 |
| 11 | 8  | 0.000000  | 0.000000  | -4.539953 |
| 12 | 6  | 0.000000  | 0.000000  | -5.664717 |

#### 16a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.418721 |
| 2  | 9  | -1.142639 | 0.659703  | -2.907360 |
| 3  | 9  | 0.000000  | 0.000000  | -4.790201 |
| 4  | 9  | 1.142639  | 0.659703  | -2.907360 |
| 5  | 9  | -0.000000 | -1.319406 | -2.907360 |
| 6  | 15 | 0.000000  | 0.000000  | 0.297256  |
| 7  | 35 | 0.000000  | 2.018203  | -0.353947 |
| 8  | 35 | 1.747815  | -1.009102 | -0.353947 |
| 9  | 35 | 0.000000  | 0.000000  | 2.453228  |
| 10 | 35 | -1.747815 | -1.009102 | -0.353947 |
| 11 | 6  | 0.000000  | 0.000000  | 6.606071  |
| 12 | 1  | 0.000000  | 0.000000  | 7.675865  |
| 13 | 7  | 0.000000  | 0.000000  | 5.462065  |

#### 16b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 4.419874  |
| 2  | 9  | 0.000000  | 0.000000  | 5.785329  |
| 3  | 9  | 0.000000  | -1.313014 | 3.887673  |
| 4  | 9  | -1.137104 | 0.656507  | 3.887673  |
| 5  | 9  | 1.137104  | 0.656507  | 3.887673  |
| 6  | 15 | 0.000000  | 0.000000  | -0.650140 |
| 7  | 35 | 0.000000  | 2.004504  | -1.426134 |
| 8  | 35 | -1.735952 | -1.002252 | -1.426134 |
| 9  | 35 | 0.000000  | 0.000000  | 1.444336  |
| 10 | 35 | 1.735952  | -1.002252 | -1.426134 |
| 11 | 6  | 0.000000  | 0.000000  | -5.509620 |
| 12 | 1  | 0.000000  | 0.000000  | -6.579572 |
| 13 | 7  | 0.000000  | 0.000000  | -4.364682 |

#### 17a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.276021 |
| 2  | 9  | -1.143039 | 0.659934  | -2.766661 |
| 3  | 9  | 0.000000  | 0.000000  | -4.648700 |
| 4  | 9  | 1.143039  | 0.659934  | -2.766661 |
| 5  | 9  | -0.000000 | -1.319868 | -2.766661 |
| 6  | 15 | 0.000000  | 0.000000  | 0.462973  |
| 7  | 35 | 0.000000  | 2.017868  | -0.203282 |
| 8  | 35 | 1.747525  | -1.008934 | -0.203282 |
| 9  | 35 | 0.000000  | 0.000000  | 2.643101  |
| 10 | 35 | -1.747525 | -1.008934 | -0.203282 |
| 11 | 7  | 0.000000  | 0.000000  | 5.371841  |
| 12 | 1  | 0.818530  | 0.472579  | 5.735614  |

|    |   |           |           |          |
|----|---|-----------|-----------|----------|
| 13 | 1 | -0.000000 | -0.945157 | 5.735614 |
| 14 | 1 | -0.818530 | 0.472579  | 5.735614 |

### 17b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 4.285042  |
| 2  | 9  | 0.000000  | 0.000000  | 5.650668  |
| 3  | 9  | 0.000000  | -1.313042 | 3.753032  |
| 4  | 9  | -1.137128 | 0.656521  | 3.753032  |
| 5  | 9  | 1.137128  | 0.656521  | 3.753032  |
| 6  | 15 | 0.000000  | 0.000000  | -0.783961 |
| 7  | 35 | 0.000000  | 2.011552  | -1.543455 |
| 8  | 35 | -1.742055 | -1.005776 | -1.543455 |
| 9  | 35 | 0.000000  | 0.000000  | 1.311096  |
| 10 | 35 | 1.742055  | -1.005776 | -1.543455 |
| 11 | 7  | 0.000000  | 0.000000  | -4.452017 |
| 12 | 1  | 0.000000  | 0.937207  | -4.838365 |
| 13 | 1  | -0.811645 | -0.468604 | -4.838365 |
| 14 | 1  | 0.811645  | -0.468604 | -4.838365 |

### 18a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.957981 |
| 2  | 9  | -1.144202 | 0.660605  | -3.461303 |
| 3  | 9  | 0.000000  | 0.000000  | -5.340787 |
| 4  | 9  | 1.144202  | 0.660605  | -3.461303 |
| 5  | 9  | -0.000000 | -1.321211 | -3.461303 |
| 6  | 15 | 0.000000  | 0.000000  | -0.057317 |
| 7  | 35 | 0.000000  | 2.005935  | -0.788205 |
| 8  | 35 | 1.737191  | -1.002968 | -0.788205 |
| 9  | 35 | 0.000000  | 0.000000  | 2.075329  |
| 10 | 35 | -1.737191 | -1.002968 | -0.788205 |
| 11 | 6  | 0.000000  | 0.000000  | 6.571108  |
| 12 | 7  | 0.000000  | 0.000000  | 7.737967  |
| 13 | 16 | 0.000000  | 0.000000  | 4.919030  |

### 18b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 4.903661  |
| 2  | 9  | 0.000000  | 0.000000  | 6.280999  |
| 3  | 9  | 0.000000  | -1.316027 | 4.389700  |
| 4  | 9  | -1.139713 | 0.658014  | 4.389700  |
| 5  | 9  | 1.139713  | 0.658014  | 4.389700  |
| 6  | 15 | 0.000000  | 0.000000  | -0.306099 |
| 7  | 35 | 0.000000  | 2.002878  | -1.053419 |
| 8  | 35 | -1.734543 | -1.001439 | -1.053419 |
| 9  | 35 | 0.000000  | 0.000000  | 1.804579  |
| 10 | 35 | 1.734543  | -1.001439 | -1.053419 |
| 11 | 6  | 0.000000  | 0.000000  | -5.718023 |
| 12 | 7  | 0.000000  | 0.000000  | -6.885541 |
| 13 | 16 | 0.000000  | 0.000000  | -4.063881 |

### 19a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -4.121483 |
| 2  | 9  | -1.145827 | 0.661544  | -3.637314 |
| 3  | 9  | 0.000000  | 0.000000  | -5.513588 |
| 4  | 9  | 1.145827  | 0.661544  | -3.637314 |
| 5  | 9  | -0.000000 | -1.323087 | -3.637314 |
| 6  | 15 | 0.000000  | 0.000000  | -0.001164 |
| 7  | 35 | 0.000000  | 2.003667  | -0.831844 |
| 8  | 35 | 1.735226  | -1.001833 | -0.831844 |
| 9  | 35 | 0.000000  | 0.000000  | 2.370734  |
| 10 | 35 | -1.735226 | -1.001833 | -0.831844 |
| 11 | 35 | 0.000000  | 0.000000  | 4.937788  |

#### 19b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -4.698140 |
| 2  | 9  | 0.000000  | 0.000000  | -6.092563 |
| 3  | 9  | 0.000000  | -1.320921 | -4.210821 |
| 4  | 9  | 1.143952  | 0.660461  | -4.210821 |
| 5  | 9  | -1.143952 | 0.660461  | -4.210821 |
| 6  | 15 | 0.000000  | 0.000000  | 0.919762  |
| 7  | 35 | 0.000000  | 2.224654  | 1.021551  |
| 8  | 35 | 1.926607  | -1.112327 | 1.021551  |
| 9  | 35 | 0.000000  | 0.000000  | -1.320027 |
| 10 | 35 | -1.926607 | -1.112327 | 1.021551  |
| 11 | 35 | 0.000000  | 0.000000  | 3.347362  |

#### 20a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.605874 |
| 2  | 9  | -1.142967 | 0.659892  | -3.094951 |
| 3  | 9  | 0.000000  | 0.000000  | -4.976724 |
| 4  | 9  | 1.142967  | 0.659892  | -3.094951 |
| 5  | 9  | -0.000000 | -1.319785 | -3.094951 |
| 6  | 15 | 0.000000  | 0.000000  | 0.171205  |
| 7  | 53 | 0.000000  | 0.000000  | 2.581967  |
| 8  | 53 | 0.000000  | 2.258394  | -0.529960 |
| 9  | 53 | 1.955826  | -1.129197 | -0.529960 |
| 10 | 53 | -1.955826 | -1.129197 | -0.529960 |
| 11 | 8  | 0.000000  | 0.000000  | 6.997183  |
| 12 | 6  | 0.000000  | 0.000000  | 5.876247  |

#### 20b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 4.902565  |
| 2  | 9  | 0.000000  | 0.000000  | 6.261302  |
| 3  | 9  | -1.134027 | 0.654731  | 4.356861  |
| 4  | 9  | 1.134027  | 0.654731  | 4.356861  |
| 5  | 9  | -0.000000 | -1.309462 | 4.356861  |
| 6  | 15 | 0.000000  | 0.000000  | -0.476976 |
| 7  | 53 | 0.000000  | 2.231154  | -1.365992 |
| 8  | 53 | 1.932236  | -1.115577 | -1.365992 |
| 9  | 53 | -1.932236 | -1.115577 | -1.365992 |
| 10 | 53 | 0.000000  | 0.000000  | 1.868253  |
| 11 | 8  | 0.000000  | 0.000000  | -5.707464 |
| 12 | 6  | 0.000000  | 0.000000  | -4.585031 |

**21a**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.607177 |
| 2  | 9  | -1.142855 | 0.659828  | -3.097785 |
| 3  | 9  | 0.000000  | 0.000000  | -4.979340 |
| 4  | 9  | 1.142855  | 0.659828  | -3.097785 |
| 5  | 9  | -0.000000 | -1.319656 | -3.097785 |
| 6  | 15 | 0.000000  | 0.000000  | 0.204422  |
| 7  | 53 | 0.000000  | 0.000000  | 2.609936  |
| 8  | 53 | 0.000000  | 2.255265  | -0.517023 |
| 9  | 53 | 1.953117  | -1.127633 | -0.517023 |
| 10 | 53 | -1.953117 | -1.127633 | -0.517023 |
| 11 | 6  | 0.000000  | 0.000000  | 6.731284  |
| 12 | 1  | 0.000000  | 0.000000  | 7.801266  |
| 13 | 7  | 0.000000  | 0.000000  | 5.587844  |

**21b**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 4.898155  |
| 2  | 9  | 0.000000  | 0.000000  | 6.258829  |
| 3  | 9  | -1.134573 | 0.655046  | 4.355766  |
| 4  | 9  | 1.134573  | 0.655046  | 4.355766  |
| 5  | 9  | -0.000000 | -1.310092 | 4.355766  |
| 6  | 15 | 0.000000  | 0.000000  | -0.501297 |
| 7  | 53 | -0.000000 | 2.233629  | -1.375504 |
| 8  | 53 | 1.934380  | -1.116815 | -1.375504 |
| 9  | 53 | -1.934380 | -1.116815 | -1.375504 |
| 10 | 53 | 0.000000  | 0.000000  | 1.846480  |
| 11 | 6  | 0.000000  | 0.000000  | -5.500794 |
| 12 | 1  | 0.000000  | 0.000000  | -6.570506 |
| 13 | 7  | 0.000000  | 0.000000  | -4.355635 |

**22a**

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -3.512854 |
| 2  | 9  | -1.143455 | 0.660174  | -3.006208 |
| 3  | 9  | 0.000000  | 0.000000  | -4.886847 |
| 4  | 9  | 1.143455  | 0.660174  | -3.006208 |
| 5  | 9  | -0.000000 | -1.320348 | -3.006208 |
| 6  | 15 | 0.000000  | 0.000000  | 0.328893  |
| 7  | 53 | 0.000000  | 0.000000  | 2.776754  |
| 8  | 53 | -0.000000 | 2.253567  | -0.410202 |
| 9  | 53 | 1.951646  | -1.126783 | -0.410202 |
| 10 | 53 | -1.951646 | -1.126783 | -0.410202 |
| 11 | 7  | 0.000000  | 0.000000  | 5.476471  |
| 12 | 1  | -0.821158 | -0.474096 | 5.833004  |
| 13 | 1  | 0.000000  | 0.948192  | 5.833004  |
| 14 | 1  | 0.821158  | -0.474096 | 5.833004  |

**22b**

|   |   |          |          |          |
|---|---|----------|----------|----------|
| 1 | 5 | 0.000000 | 0.000000 | 4.788698 |
| 2 | 9 | 0.000000 | 0.000000 | 6.149100 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 3  | 9  | -1.134512 | 0.655011  | 4.245888  |
| 4  | 9  | 1.134512  | 0.655011  | 4.245888  |
| 5  | 9  | -0.000000 | -1.310021 | 4.245888  |
| 6  | 15 | 0.000000  | 0.000000  | -0.608840 |
| 7  | 53 | -0.000000 | 2.243796  | -1.461270 |
| 8  | 53 | 1.943185  | -1.121898 | -1.461270 |
| 9  | 53 | -1.943185 | -1.121898 | -1.461270 |
| 10 | 53 | 0.000000  | 0.000000  | 1.738971  |
| 11 | 7  | 0.000000  | 0.000000  | -4.347346 |
| 12 | 1  | -0.000000 | 0.939262  | -4.727934 |
| 13 | 1  | -0.813425 | -0.469631 | -4.727934 |
| 14 | 1  | 0.813425  | -0.469631 | -4.727934 |

### 23a

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | -4.087563 |
| 2  | 9  | -1.144719 | 0.660904  | -3.593439 |
| 3  | 9  | 0.000000  | 0.000000  | -5.471739 |
| 4  | 9  | 1.144719  | 0.660904  | -3.593439 |
| 5  | 9  | -0.000000 | -1.321807 | -3.593439 |
| 6  | 15 | 0.000000  | 0.000000  | -0.040449 |
| 7  | 53 | 0.000000  | 0.000000  | 2.348911  |
| 8  | 53 | 0.000000  | 2.235455  | -0.866219 |
| 9  | 53 | 1.935961  | -1.117728 | -0.866219 |
| 10 | 53 | -1.935961 | -1.117728 | -0.866219 |
| 11 | 6  | 0.000000  | 0.000000  | 6.855393  |
| 12 | 7  | 0.000000  | 0.000000  | 8.021453  |
| 13 | 16 | 0.000000  | 0.000000  | 5.204194  |

### 23b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 5.279922  |
| 2  | 9  | 0.000000  | 0.000000  | 6.653052  |
| 3  | 9  | -1.137689 | 0.656845  | 4.757620  |
| 4  | 9  | 1.137689  | 0.656845  | 4.757620  |
| 5  | 9  | -0.000000 | -1.313690 | 4.757620  |
| 6  | 15 | 0.000000  | 0.000000  | -0.255324 |
| 7  | 53 | -0.000000 | 2.234301  | -1.094195 |
| 8  | 53 | 1.934961  | -1.117150 | -1.094195 |
| 9  | 53 | -1.934961 | -1.117150 | -1.094195 |
| 10 | 53 | 0.000000  | 0.000000  | 2.106009  |
| 11 | 6  | 0.000000  | 0.000000  | -5.752983 |
| 12 | 7  | 0.000000  | 0.000000  | -6.920725 |
| 13 | 16 | 0.000000  | 0.000000  | -4.098845 |

### 24a

|   |    |           |           |           |
|---|----|-----------|-----------|-----------|
| 1 | 5  | 0.000000  | 0.000000  | -4.262085 |
| 2 | 9  | -1.145680 | 0.661458  | -3.777027 |
| 3 | 9  | 0.000000  | 0.000000  | -5.653757 |
| 4 | 9  | 1.145680  | 0.661458  | -3.777027 |
| 5 | 9  | -0.000000 | -1.322917 | -3.777027 |
| 6 | 15 | 0.000000  | 0.000000  | -0.022196 |
| 7 | 53 | 0.000000  | 0.000000  | 2.611550  |
| 8 | 53 | 0.000000  | 2.226422  | -0.933874 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 9  | 53 | 1.928138  | -1.113211 | -0.933874 |
| 10 | 53 | -1.928138 | -1.113211 | -0.933874 |
| 11 | 35 | 0.000000  | 0.000000  | 5.273737  |

## 24b

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 1  | 5  | 0.000000  | 0.000000  | 5.315683  |
| 2  | 9  | 0.000000  | 0.000000  | 6.694393  |
| 3  | 9  | -1.139422 | 0.657845  | 4.802955  |
| 4  | 9  | 1.139422  | 0.657845  | 4.802955  |
| 5  | 9  | -0.000000 | -1.315691 | 4.802955  |
| 6  | 15 | 0.000000  | 0.000000  | -0.308880 |
| 7  | 53 | 0.000000  | 2.264924  | -1.131426 |
| 8  | 53 | 1.961482  | -1.132462 | -1.131426 |
| 9  | 53 | -1.961482 | -1.132462 | -1.131426 |
| 10 | 53 | 0.000000  | 0.000000  | 2.062374  |
| 11 | 35 | 0.000000  | 0.000000  | -4.036675 |