

# Structures and Spectroscopy of protonated ammonia clusters at different Temperatures

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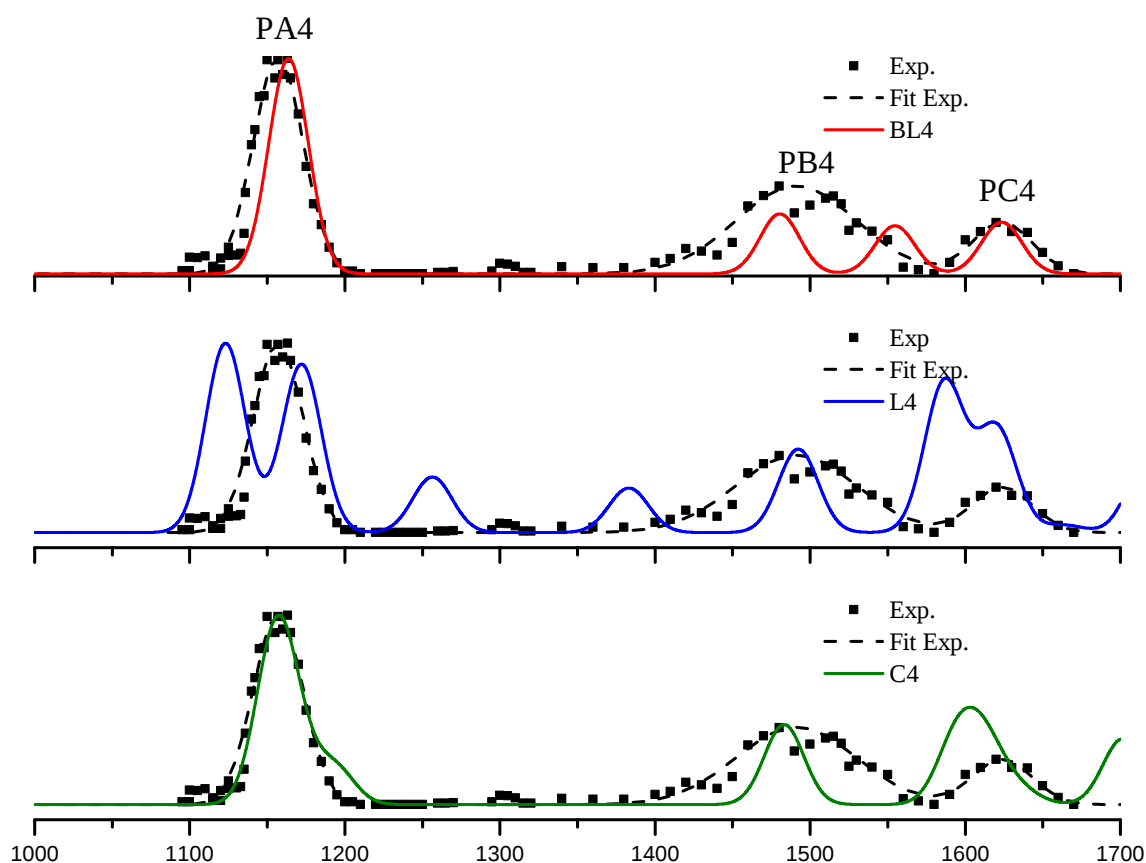
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## SUPPORTING INFORMATION:

**KEYWORDS:** protonated ammonia clusters, interaction energies, relative stability, hydrogen bond network.

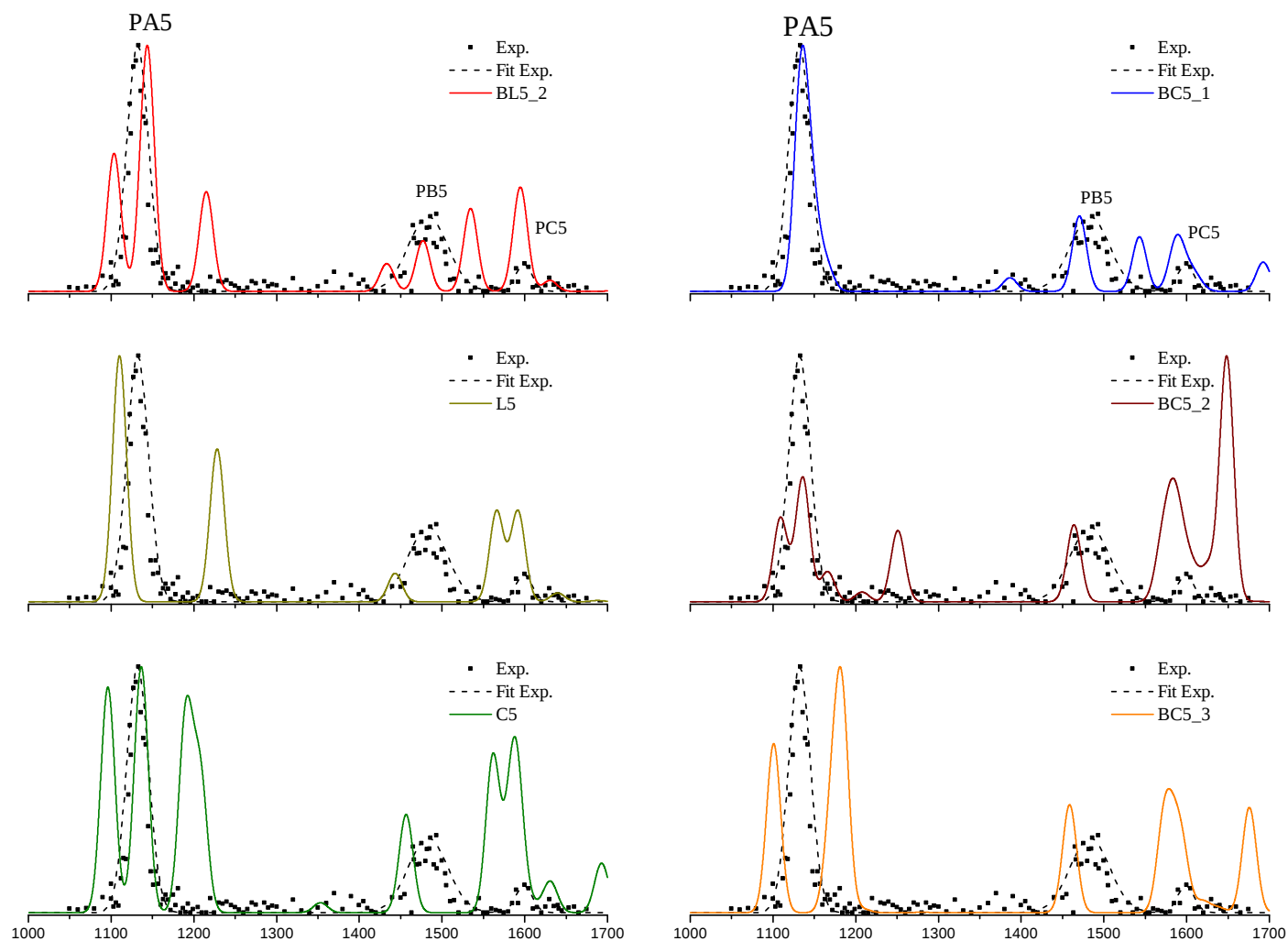
### 1 Infrared Spectra of Some Isomers of Protonated Ammonia Tetramer



**Fig. S 1** Comparison of the experimental IR spectrum for the protonated ammonia tetramer with the calculated scaled harmonic IR spectrum of isomers of  $\text{NH}_4^+(\text{NH}_3)_3$ , except **BL4**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factors of 0.943 and 0.965 were applied for  $\omega < 1400$  and  $\omega \in [1400 - 1700]$ , respectively. The same FWHM of  $30\text{cm}^{-1}$  is used for all the calculated absorption bands. Experimental data courtesy of Kensuke Tono.

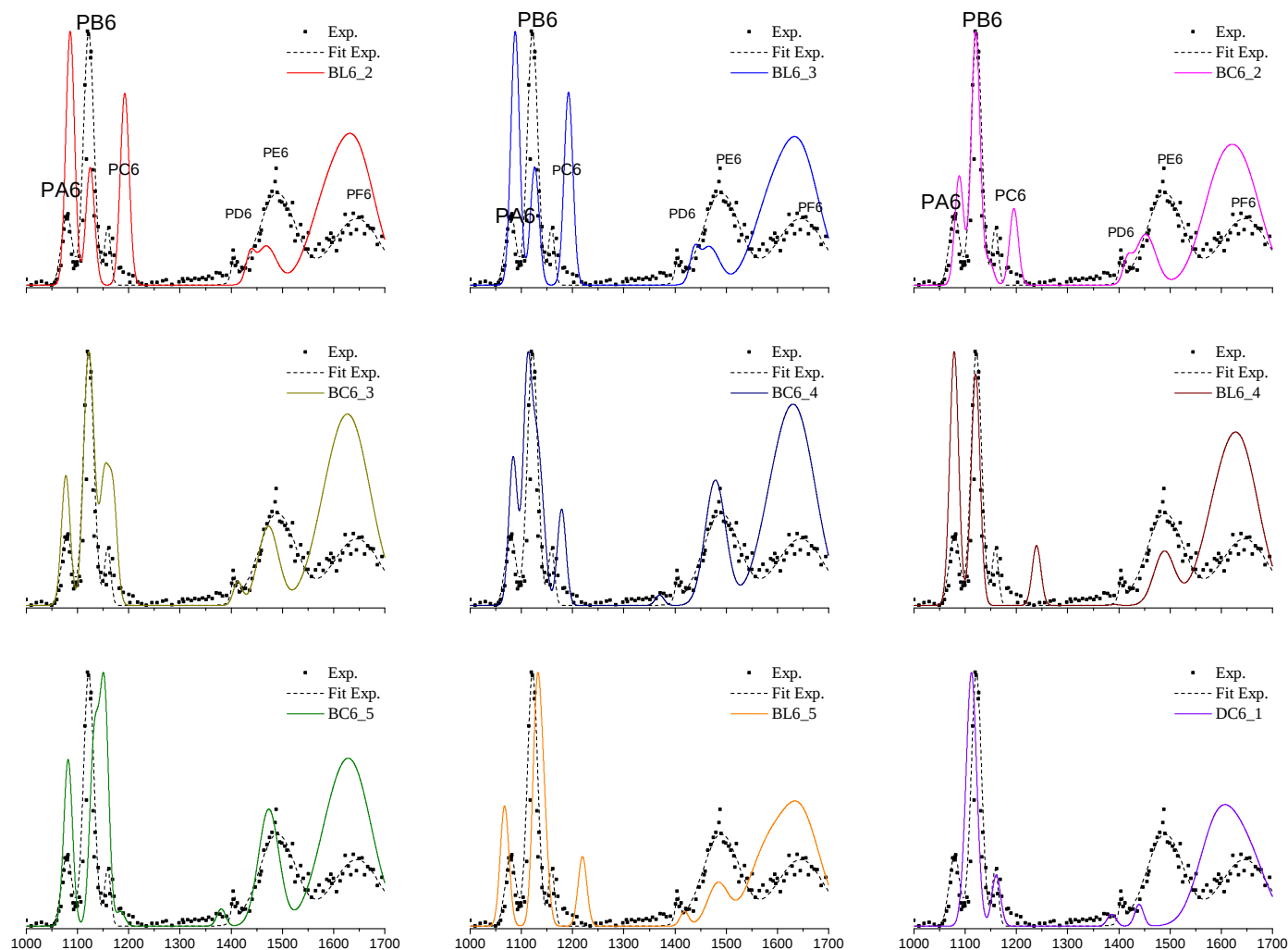
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## 2 Infrared Spectra of Some Isomers of Protonated Ammonia Pentamer

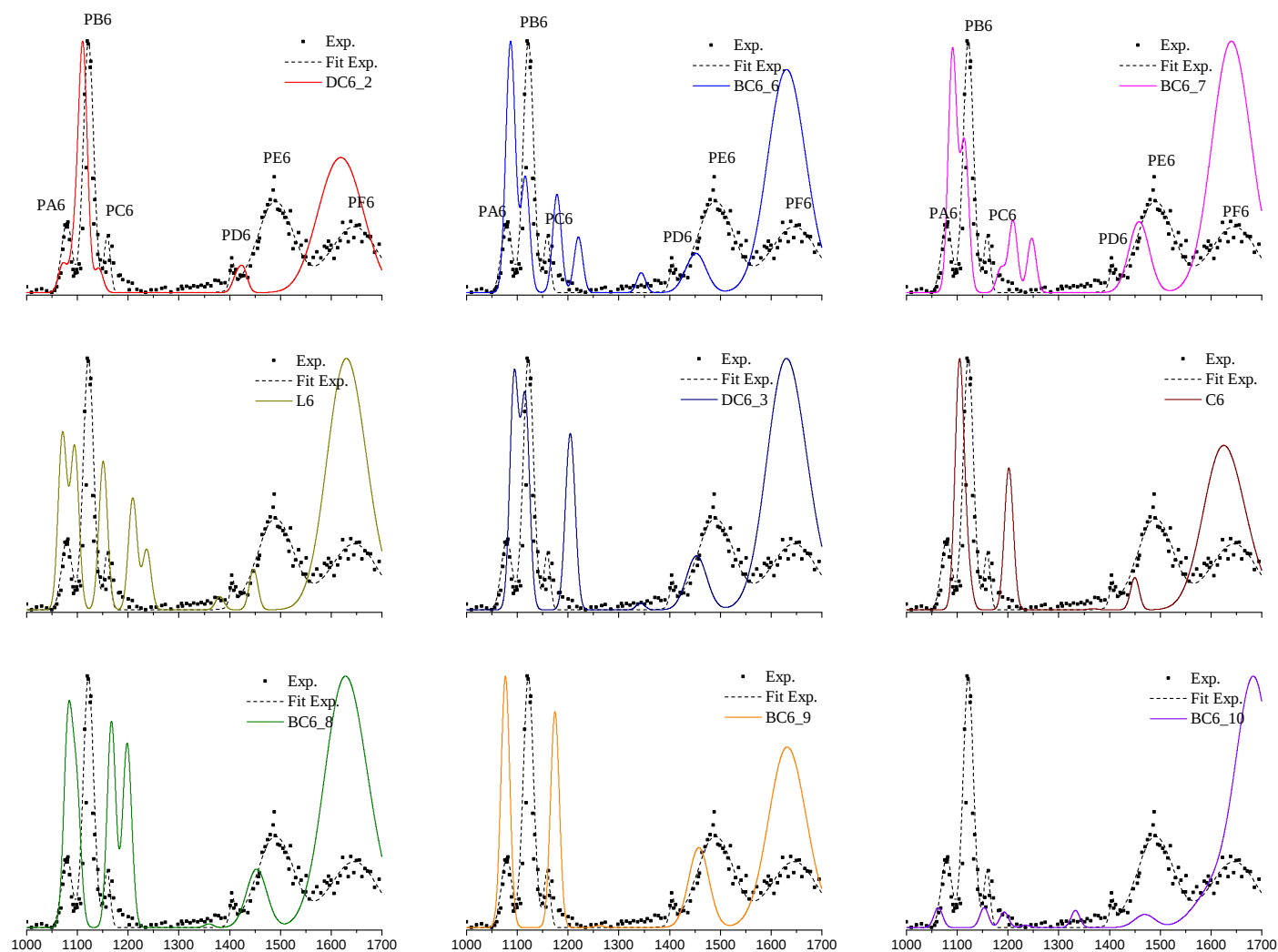


**Fig. S 2** Comparison of the experimental IR spectrum for the protonated ammonia pentamer with the calculated scaled harmonic IR spectrum of the isomers of  $\text{NH}_4^+(\text{NH}_3)_4$ , except **BL5**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factors of 0.939 and 0.949 were applied for  $\omega < 1400$  and  $\omega \in [1400 - 1700]$ , respectively. The same FWHM of  $20\text{ cm}^{-1}$  is used for all the calculated absorption bands. Experimental data courtesy of Kensuke Tono.

## 3 Infrared Spectra of Some Isomers of Protonated Ammonia Hexamer

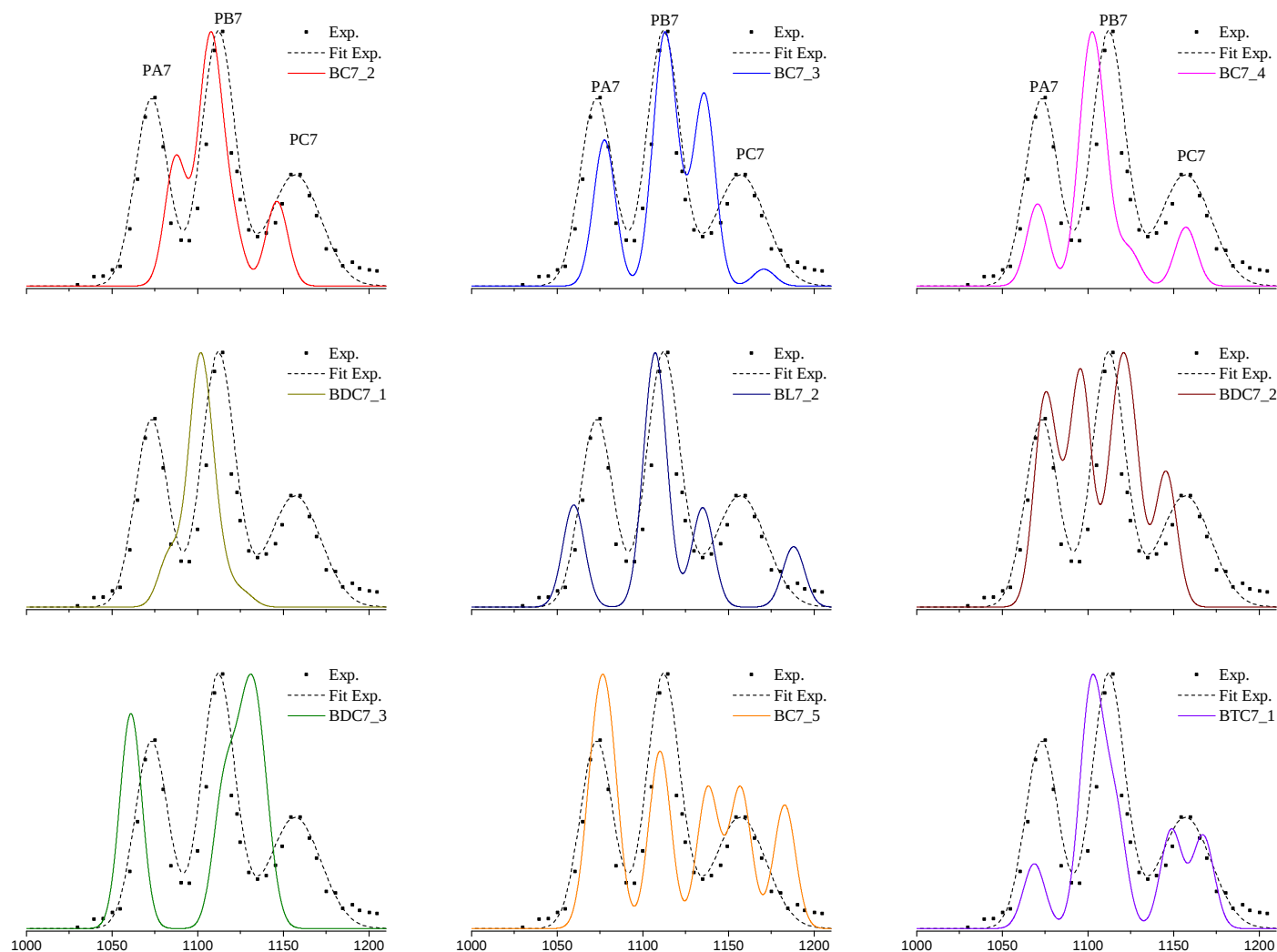


**Fig. S 3** Experimental IR spectrum for the protonated ammonia hexamer with the calculated scaled harmonic IR spectra of the isomers **BL6.2**, **BL6.3**, **BC6.2**, **BC6.3**, **BC6.4**, **BL6.4**, **BC6.5**, **BL6.5** and **DC6.2**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factors of 0.931, 0.949 and 0.977 were applied for  $\omega < 1400$ ,  $\omega \in [1400 - 1600]$  and  $\omega \in [1600 - 1700]$ , respectively. The corresponding FWHM applied for the corresponding calculated absorption bands are respectively 20, 47 and  $82\text{ cm}^{-1}$ . Experimental data courtesy of Kensuke Tono.

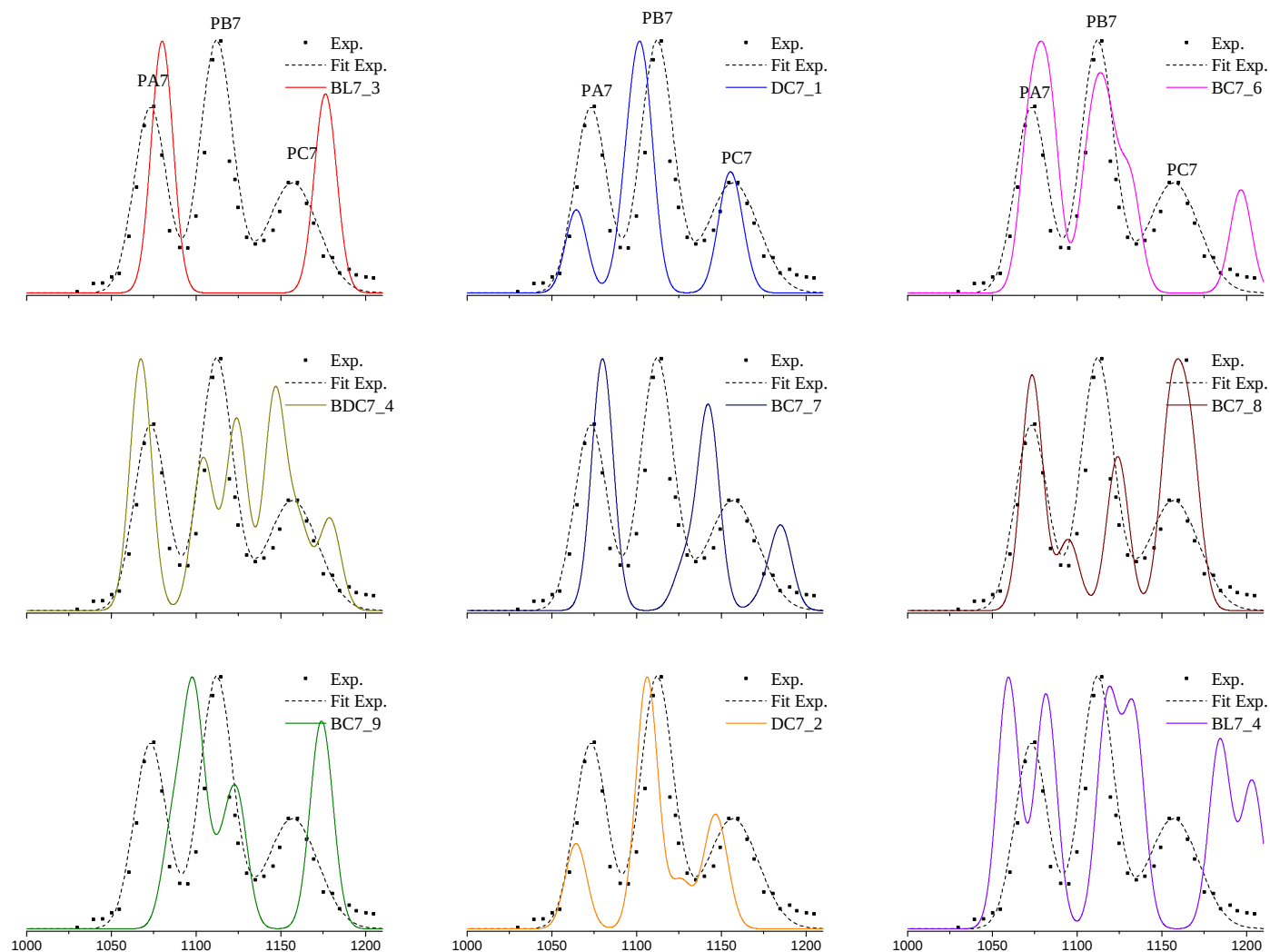


**Fig. S 4** Experimental IR spectrum for the protonated ammonia hexamer with the calculated scaled harmonic IR spectra of the isomers **DC6.2**, **BC6.6**, **BC6.7**, **L6**, **DC6.3**, **C6**, **BC6.8**, **BC6.9** and **BC6.10**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factors of 0.931, 0.949 and 0.977 were applied for  $\omega < 1400$ ,  $\omega \in [1400 - 1600]$  and  $\omega \in [1600 - 1700]$ , respectively. The corresponding FWHM applied for the corresponding calculated absorption bands are respectively 20, 47 and 82  $\text{cm}^{-1}$ . Experimental data courtesy of Kensuke Tono.

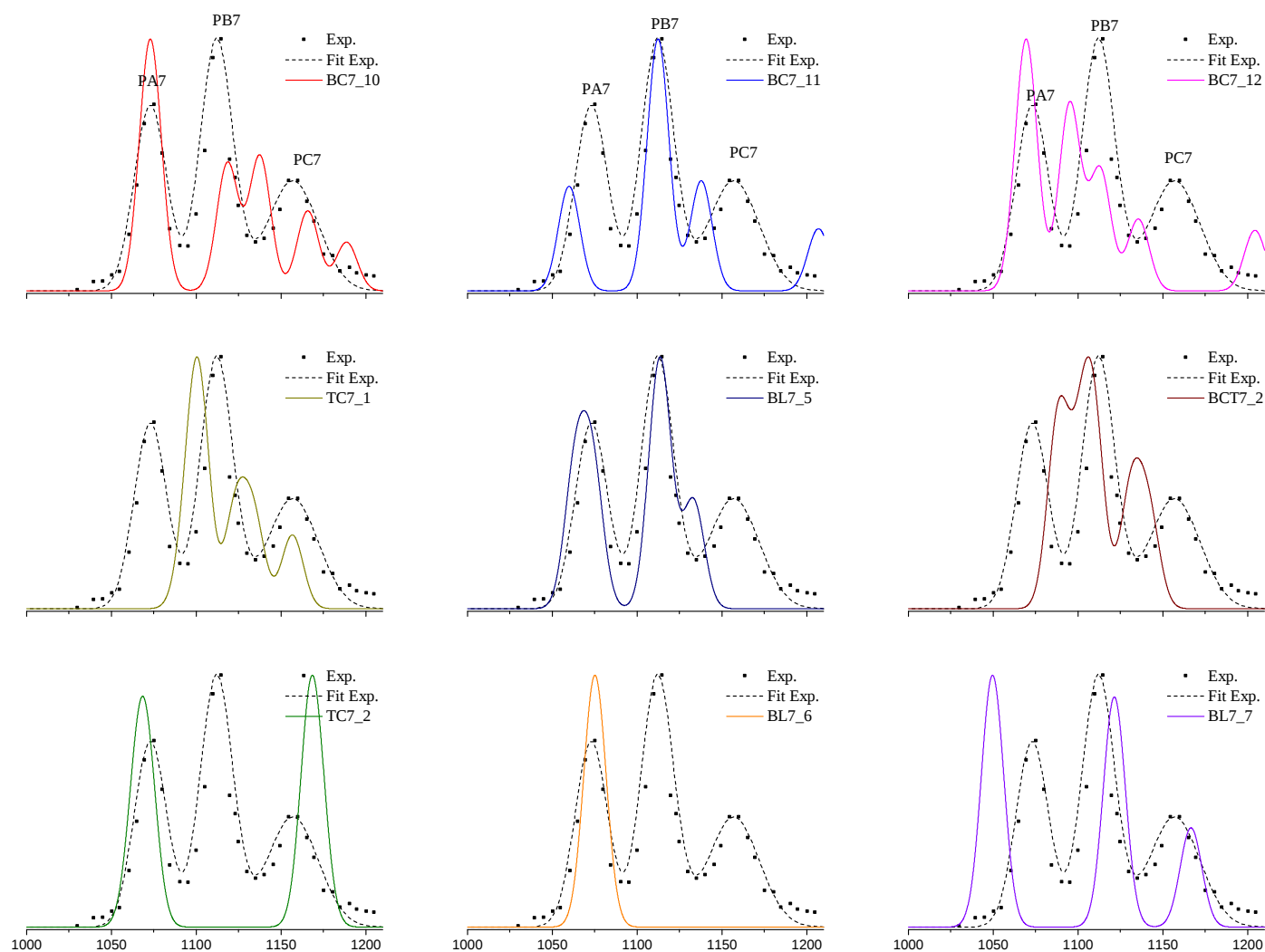
## 4 Infrared Spectra of Some Isomers of Protonated Ammonia Heptamer



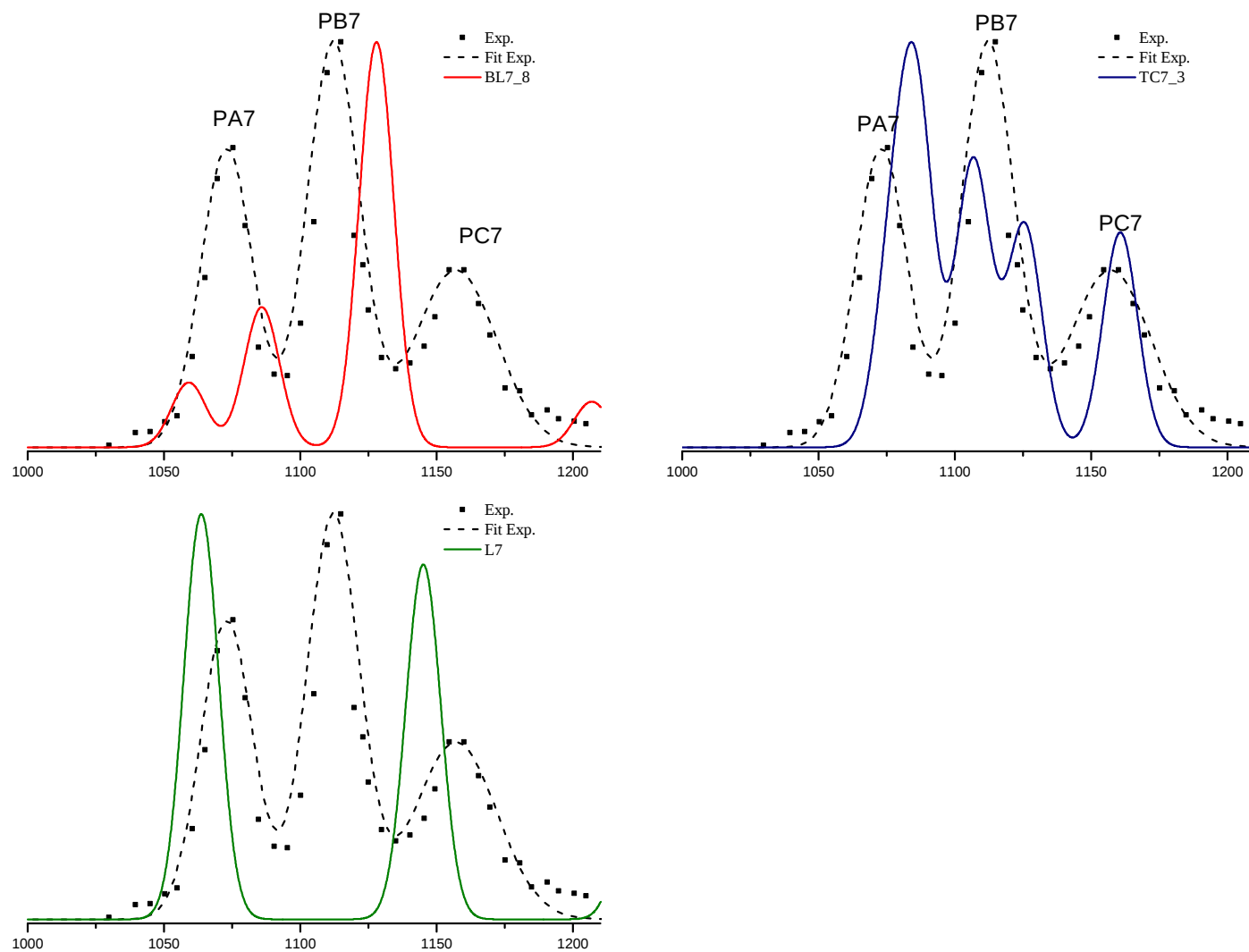
**Fig. S 5** Experimental IR spectrum for the protonated ammonia heptamer with the calculated scaled harmonic IR spectra of the isomers **BC7\_2**, **BC7\_3**, **BC7\_4**, **BDC7\_1**, **BL7\_2**, **BDC7\_2**, **BDC7\_3**, **BC7\_5** and **BTC7\_1**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.930 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands. Experimental data courtesy of Kensuke Tono.



**Fig. S 6** Experimental IR spectrum for the protonated ammonia heptamer with the calculated scaled harmonic IR spectra of the isomers **BL7\_3**, **DC7\_1**, **BC7\_6**, **BDC7\_4**, **BC7\_7**, **BC7\_8**, **BC7\_9**, **DC7\_2** and **BL7\_4**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.930 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands Experimental data courtesy of Kensuke Tono.

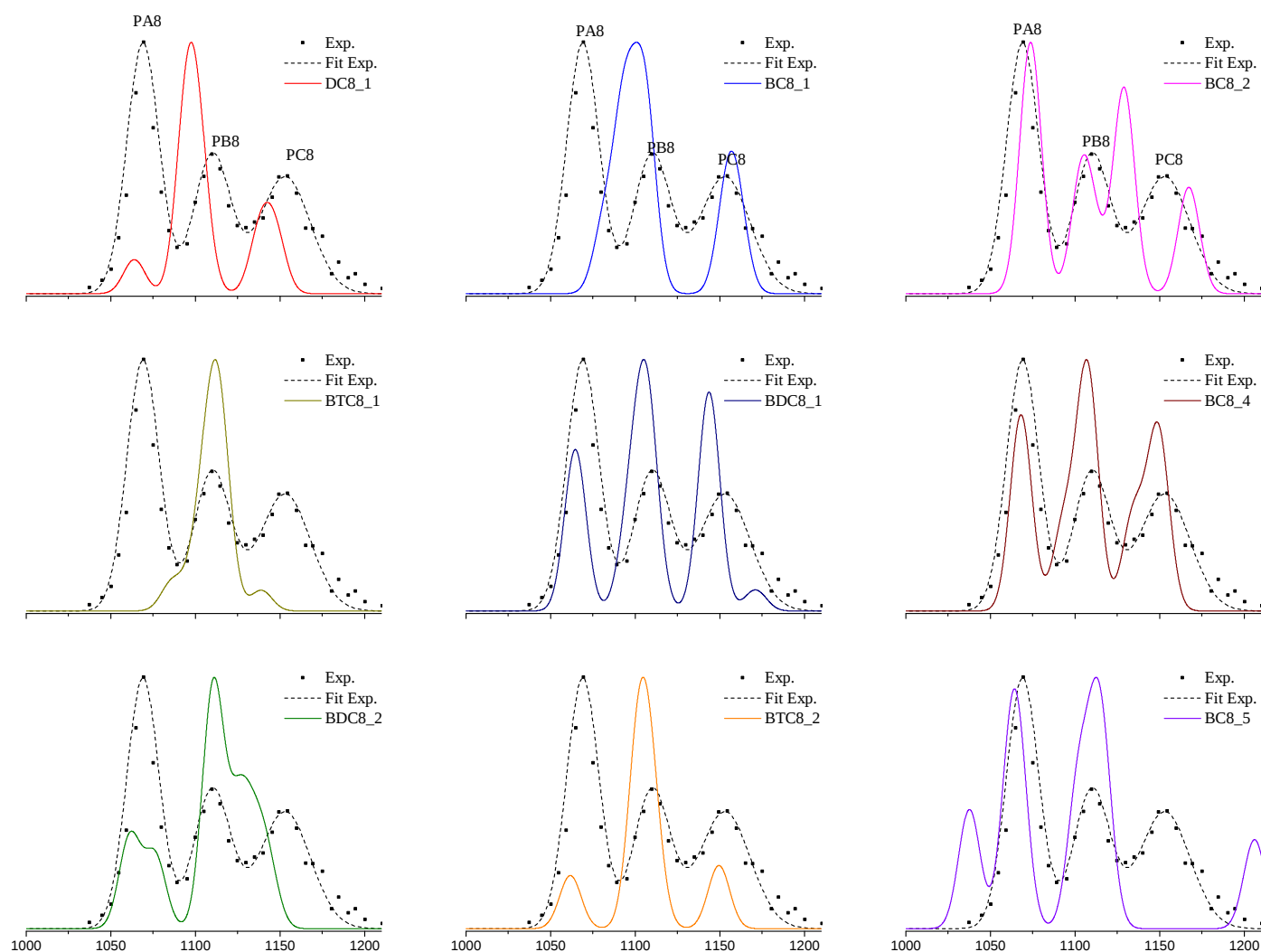


**Fig. S 7** Experimental IR spectrum for the protonated ammonia heptamer with the calculated scaled harmonic IR spectra of the isomers **BC7\_10**, **BC7\_11**, **BC7\_12**, **TC7\_1**, **BL7\_5**, **BTC7\_2**, **TC7\_2**, **BL7\_6** and **BL7\_7**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.930 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands. Experimental data courtesy of Kensuke Tono.

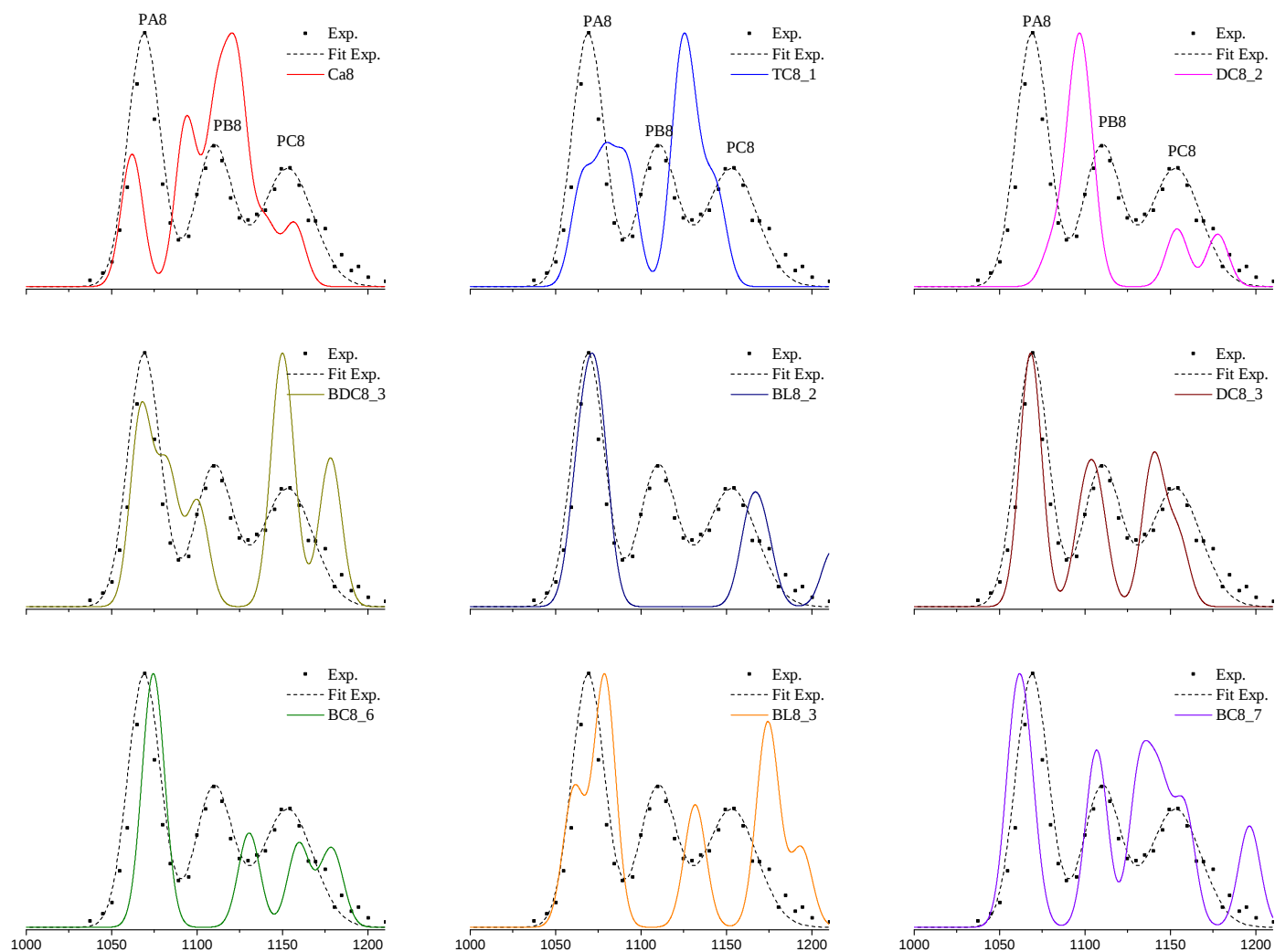


**Fig. S 8** Experimental IR spectrum for the protonated ammonia heptamer with the calculated scaled harmonic IR spectra of the isomers **BL7\_8**, **TC7\_3** and **L7**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.930 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands. Experimental data courtesy of Kensuke Tono.

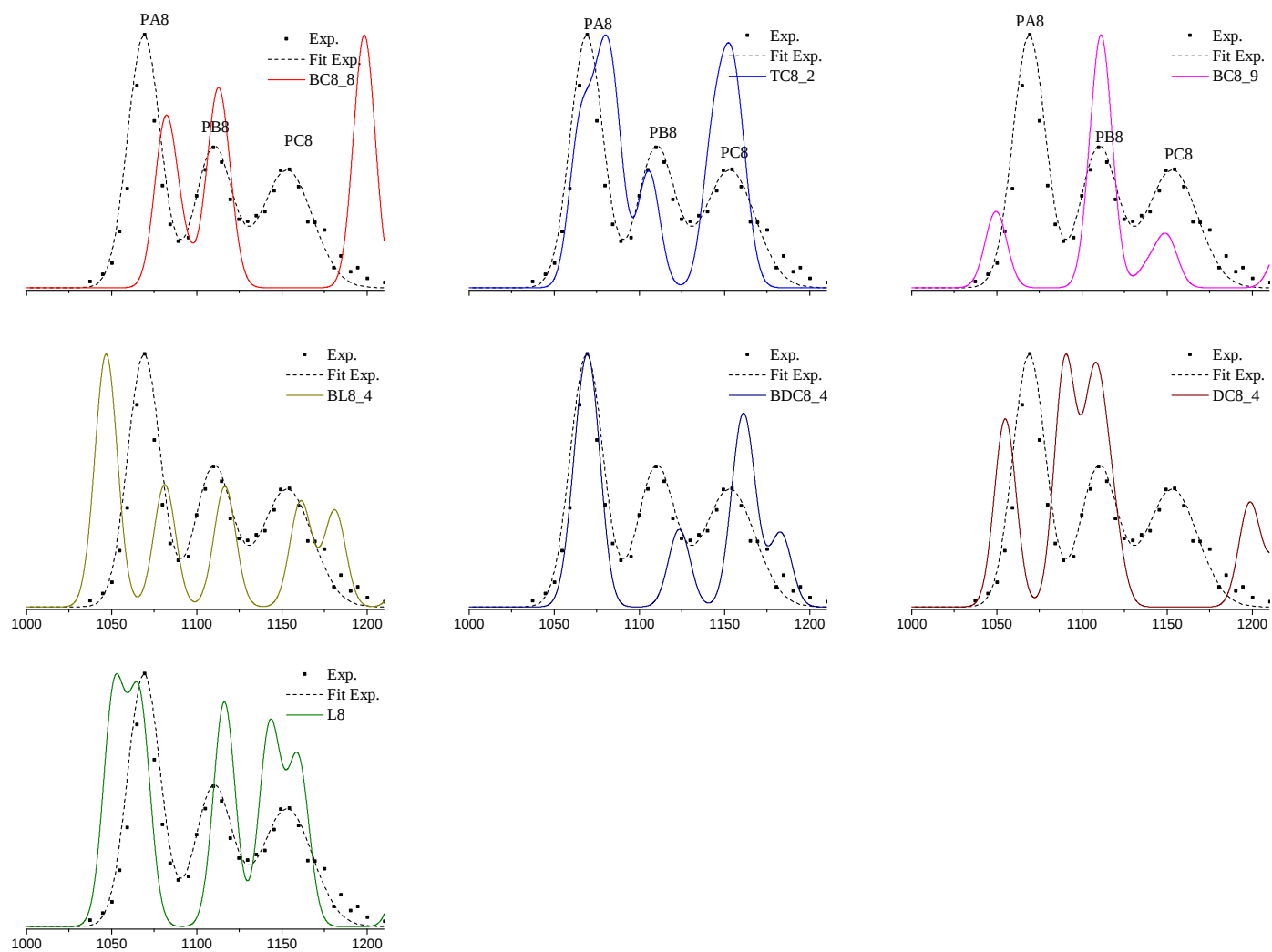
## 5 Infrared Spectra of Some Isomers of Protonated Ammonia Octamer



**Fig. S 9** Experimental IR spectrum for the protonated ammonia octamer with the calculated scaled harmonic IR spectra of the isomers **DC8\_1**, **BC8\_1**, **BC8\_2**, **BTC8\_1**, **BDC8\_1**, **BC8\_4**, **BDC8\_2**, **BTC8\_2** and **BC8\_5**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.932 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands. Experimental data courtesy of Kensuke Tono.



**Fig. S 10** Experimental IR spectrum for the protonated ammonia octamer with the calculated scaled harmonic IR spectra of the isomers **Ca8**, **TC8\_1**, **DC8\_2**, **BDC8\_3**, **BL8\_2**, **DC8\_3**, **BC8\_6**, **BL8\_3** and **BC8\_7**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.932 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands. Experimental data courtesy of Kensuke Tono.



**Fig. S 11** Experimental IR spectrum for the protonated ammonia octamer with the calculated scaled harmonic IR spectra of the isomers **BC8\_8**, **TC8\_2**, **BC8\_9**, **BL8\_4**, **BDC8\_4**, **DC8\_4** and **L8**. The calculated IR spectrum were performed at the M062X/6-31++G(d,p) level of theory. The optimized scale factor of 0.932 has been applied for the calculated IR frequencies and the FWHM of  $15\text{ cm}^{-1}$  has been applied for the calculated absorption bands. Experimental data courtesy of Kensuke Tono.

6 Thermochemistry of the protonated ammonia clusters

**Table 1** Experimental enthalpies, Experimental entropies and their averages used in the manuscript. The enthalpies are reported in kJ mol<sup>−1</sup> while the entropies are reported in J mol<sup>−1</sup> K<sup>−1</sup>

| n | Individual Δ <i>H</i>                                                                            | Av. Δ <i>H</i> | Individual Δ <i>S</i>                                                                          | Av. Δ <i>S</i> |
|---|--------------------------------------------------------------------------------------------------|----------------|------------------------------------------------------------------------------------------------|----------------|
| 1 | 107 <sup>1</sup> , 106 <sup>2</sup> , 104 <sup>3</sup> , 113 <sup>4</sup>                        | 107 ± 6        | 110 <sup>1</sup> , 102 <sup>2</sup> , 108 <sup>3</sup> , 122 <sup>4</sup>                      | 111 ± 10       |
| 2 | 72.4 <sup>2</sup> , 67.8 <sup>5</sup> , 70.7 <sup>6</sup> , 71 <sup>7</sup> , 65.7 <sup>3</sup>  | 70 ± 5         | 100 <sup>2</sup> , 99.2 <sup>5</sup> , 104 <sup>6</sup> , 112 <sup>7</sup> , 95.8 <sup>3</sup> | 102 ± 10       |
| 3 | 59.4 <sup>2</sup> , 56.5 <sup>5</sup> , 55.2 <sup>8</sup> , 57.7 <sup>3</sup> , 29 <sup>9</sup>  | 50 ± 20        | 106 <sup>2</sup> , 105 <sup>5</sup> , 101 <sup>8</sup> , 108 <sup>3</sup>                      | 105 ± 5        |
| 4 | 49.4 <sup>2</sup> , 49.0 <sup>5</sup> , 52.3 <sup>3</sup> , 50 <sup>9</sup> , 54.0 <sup>10</sup> | 51 ± 4         | 113 <sup>2</sup> , 117 <sup>5</sup> , 123 <sup>3</sup>                                         | 118 ± 8        |
| 5 | 29 <sup>5</sup> , 31 <sup>7</sup> , 30 <sup>9</sup>                                              | 30 ± 1         | 90 <sup>5</sup> , 100 <sup>7</sup> , 130 <sup>6</sup>                                          | 107 ± 23       |

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Table S1: Per ammonia binding energies of protonated ammonia clusters.

| n | (a)   | (b)   | (c)   | (d)   | (e)   |
|---|-------|-------|-------|-------|-------|
| 2 | -23,2 | -28,2 | -29,2 | -26,0 | -22,8 |
| 3 | -19,9 | -22,4 | -22,8 | -21,6 | -19,9 |
| 4 | -18,5 | -20,0 | -19,7 | -18,9 | -17,7 |
| 5 | -17,1 | -18,2 | -17,2 | -16,8 | -16,1 |
| 6 | -15,1 | -16,1 | -14,6 | -14,8 | -14,0 |
| 7 | -13,4 | -14,6 | -12,9 | -13,3 | -12,5 |
| 8 | -12,7 | -13,5 | -11,6 |       |       |
| 9 | -11,9 | -12,6 | -10,5 |       |       |

(a) This work at MP2/6-31++g\*\* and BSSE corrected

(b) This work at M06-2X/6-31++g\*\* and BSSE corrected

(c) Results from Fouqueau and Meuwly (ref.15) at B3LYP/6-31G\*\*

(d) Wang et al.(ref.13) at B3LYP/6-31+G\* and BSSE corrected

(e) Wang et al.(ref.13) at MP2/6-31+G\* and BSSE corrected

## Cartesian coordinates of the protonated ammonia dimer

Cartesian coordinates of : L2

| Atomic number (AN) and Cartesian coordinates |           |           |           |
|----------------------------------------------|-----------|-----------|-----------|
| AN                                           | X         | Y         | Z         |
| 7                                            | -1.309826 | 0.000000  | 0.000005  |
| 1                                            | -1.677357 | 0.829293  | 0.469595  |
| 1                                            | -1.677296 | -0.007940 | -0.953006 |
| 1                                            | -0.095362 | -0.000005 | 0.000043  |
| 1                                            | -1.677387 | -0.821338 | 0.483356  |
| 7                                            | 1.314599  | 0.000000  | 0.000005  |
| 1                                            | 1.697974  | 0.813522  | -0.481850 |
| 1                                            | 1.698059  | 0.010517  | 0.945424  |
| 1                                            | 1.697961  | -0.824043 | -0.463633 |

## Cartesian coordinates of the protonated ammonia trimer

Cartesian coordinates of : P\_NH3\_N3\_1.log

| Atomic number (AN) and Cartesian coordinates |           |           |           |
|----------------------------------------------|-----------|-----------|-----------|
| AN                                           | X         | Y         | Z         |
| 7                                            | 0.000000  | 1.027300  | 0.000000  |
| 1                                            | 0.894642  | 0.419774  | 0.000000  |
| 1                                            | 0.000000  | 1.627113  | -0.825605 |
| 1                                            | -0.894642 | 0.419774  | 0.000000  |
| 1                                            | 0.000000  | 1.627113  | 0.825604  |
| 7                                            | -2.327611 | -0.501497 | 0.000000  |
| 1                                            | -3.161581 | 0.083141  | 0.000086  |
| 1                                            | -2.406582 | -1.107486 | -0.814496 |
| 1                                            | -2.406502 | -1.107611 | 0.814410  |
| 7                                            | 2.327611  | -0.501497 | 0.000000  |
| 1                                            | 3.161581  | 0.083141  | -0.000072 |
| 1                                            | 2.406576  | -1.107496 | 0.814489  |
| 1                                            | 2.406509  | -1.107601 | -0.814418 |

Cartesian coordinates of the protonated ammonia tetramer

Cartesian coordinates of : BL4

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.001049 | -0.000545 | 0.656845  |
| 1  | -0.997526 | -0.115172 | 0.320172  |
| 1  | -0.000616 | -0.001794 | 1.676271  |
| 1  | 0.596486  | -0.805522 | 0.318662  |
| 1  | 0.397596  | 0.920020  | 0.320865  |
| 7  | 1.631949  | -2.198117 | -0.207623 |
| 1  | 1.292498  | -3.090186 | 0.145307  |
| 1  | 1.681328  | -2.292796 | -1.219487 |
| 1  | 2.592514  | -2.112081 | 0.117118  |
| 7  | -2.720960 | -0.312661 | -0.207657 |
| 1  | -3.175830 | -1.107305 | 0.236433  |
| 1  | -3.291238 | 0.500490  | 0.014026  |
| 1  | -2.810784 | -0.457980 | -1.210699 |
| 7  | 1.089638  | 2.511277  | -0.207251 |
| 1  | 0.531733  | 3.303073  | 0.104795  |
| 1  | 1.159001  | 2.593619  | -1.219063 |
| 1  | 2.027794  | 2.665952  | 0.155400  |

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Cartesian coordinates of : L4

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.929603 | 0.922133  | -0.015265 |
| 1  | 0.210967  | -0.136376 | -0.014993 |
| 1  | -0.893890 | 1.526437  | -0.834204 |
| 1  | -1.870539 | 0.488564  | -0.005828 |
| 1  | -0.883334 | 1.538881  | 0.793796  |
| 7  | -3.729913 | -0.237470 | 0.014232  |
| 1  | -3.935380 | -0.932107 | -0.699143 |
| 1  | -4.001938 | -0.650198 | 0.902752  |
| 1  | -4.371631 | 0.534676  | -0.148310 |
| 7  | 1.027465  | -0.916911 | -0.014968 |
| 1  | 1.996266  | -0.473852 | -0.003792 |
| 1  | 0.927769  | -1.516596 | 0.803755  |
| 1  | 0.940759  | -1.503326 | -0.844714 |
| 7  | 3.622707  | 0.229272  | 0.015043  |
| 1  | 3.804901  | 0.820435  | -0.793137 |
| 1  | 4.349631  | -0.483268 | 0.015235  |
| 1  | 3.791833  | 0.807563  | 0.835288  |

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Cartesian coordinates of : C4

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.208089 | -0.019216 | -0.000004 |
| 1  | -2.801080 | -0.027529 | 0.828821  |
| 1  | -1.553526 | 0.841149  | -0.000002 |
| 1  | -1.523570 | -0.863296 | -0.000002 |
| 1  | -2.801075 | -0.027529 | -0.828832 |
| 7  | -0.186776 | -1.865731 | 0.000003  |
| 1  | 0.648472  | -1.272364 | 0.000003  |
| 1  | -0.128749 | -2.472109 | 0.815145  |
| 1  | -0.128746 | -2.472114 | -0.815134 |
| 7  | -0.216488 | 1.877705  | 0.000003  |
| 1  | -0.163824 | 2.484408  | -0.815117 |
| 1  | -0.163827 | 2.484403  | 0.815127  |
| 1  | 0.621891  | 1.291092  | 0.000003  |
| 7  | 2.507084  | 0.000402  | -0.000003 |

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1      2.872543      0.492036      0.813230
1      2.978833     -0.902289      0.000004
1      2.872536      0.492021     -0.813248
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Cartesian coordinates of the protonated ammonia pentamer

Cartesian coordinates of : BL5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.017734  | -0.000929 | -0.059447 |
| 1  | 0.026138  | 0.014890  | 0.986029  |
| 1  | 1.000497  | 0.018428  | -0.416071 |
| 1  | -0.456510 | -0.871892 | -0.390951 |
| 1  | -0.499355 | 0.834895  | -0.416355 |
| 7  | -1.319294 | -2.452809 | -0.991431 |
| 1  | -0.863154 | -3.297275 | -0.654771 |
| 1  | -2.286827 | -2.508966 | -0.682784 |
| 1  | -1.338987 | -2.524353 | -2.005838 |
| 7  | -1.439535 | 2.352510  | -1.062308 |
| 1  | -2.408322 | 2.370481  | -0.753002 |
| 1  | -1.024980 | 3.228068  | -0.752336 |
| 1  | -1.463871 | 2.392554  | -2.078351 |
| 7  | 2.785820  | 0.053481  | -1.060638 |
| 1  | 3.300957  | 0.867592  | -0.734422 |
| 1  | 3.321490  | -0.759579 | -0.766444 |
| 1  | 2.833574  | 0.074085  | -2.076422 |
| 7  | 0.041142  | 0.043842  | 2.884417  |
| 1  | -0.892746 | -0.021989 | 3.281981  |
| 1  | 0.450404  | 0.896943  | 3.257609  |
| 1  | 0.574792  | -0.725700 | 3.281356  |

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Cartesian coordinates of : BL5\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.811438 | -0.001158 | -0.503117 |
| 1  | 0.070837  | -0.068587 | 0.117528  |
| 1  | -0.524373 | -0.002399 | -1.480809 |
| 1  | -1.440150 | -0.827779 | -0.336855 |
| 1  | -1.330378 | 0.892250  | -0.307227 |
| 7  | -2.540113 | -2.293694 | -0.073532 |
| 1  | -2.114853 | -3.162150 | -0.389674 |
| 1  | -2.775431 | -2.431740 | 0.906448  |
| 1  | -3.424268 | -2.212688 | -0.570155 |
| 7  | 1.474005  | -0.175777 | 1.069909  |
| 1  | 1.529143  | -1.053621 | 1.581677  |
| 1  | 2.336607  | -0.108454 | 0.509000  |
| 1  | 1.524083  | 0.560644  | 1.770417  |
| 7  | -2.239803 | 2.475860  | 0.006222  |
| 1  | -1.656617 | 3.296268  | -0.141282 |
| 1  | -2.586633 | 2.540106  | 0.960347  |
| 1  | -3.049236 | 2.589522  | -0.599447 |
| 7  | 4.120725  | -0.009010 | -0.503281 |
| 1  | 4.865710  | 0.000255  | 0.188544  |
| 1  | 4.250730  | 0.821252  | -1.074819 |
| 1  | 4.301202  | -0.806431 | -1.107100 |

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Cartesian coordinates of : BC5\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.250133 | 0.004124  | -0.854040 |
| 1  | -0.631180 | -0.829445 | -0.633305 |
| 1  | -1.491550 | 0.003084  | -1.843559 |
| 1  | -2.134566 | 0.000959  | -0.281050 |
| 1  | -0.640026 | 0.841072  | -0.634443 |
| 7  | -3.708171 | -0.003677 | 0.656480  |
| 1  | -4.260218 | 0.834407  | 0.488819  |
| 1  | -3.567744 | -0.056526 | 1.662644  |
| 1  | -4.303108 | -0.791290 | 0.409594  |
| 7  | 3.374547  | -0.015227 | 0.500061  |
| 1  | 3.802008  | -0.921662 | 0.679631  |
| 1  | 3.931817  | 0.406376  | -0.239943 |
| 1  | 3.551558  | 0.537042  | 1.336509  |
| 7  | 0.744140  | -1.872236 | -0.186148 |
| 1  | 1.535466  | -1.260919 | 0.031112  |
| 1  | 0.576629  | -2.451308 | 0.632866  |
| 1  | 1.043475  | -2.501211 | -0.927218 |
| 7  | 0.753554  | 1.881943  | -0.179499 |
| 1  | 1.062638  | 2.510800  | -0.916511 |
| 1  | 1.533392  | 1.256084  | 0.033843  |
| 1  | 0.593847  | 2.458044  | 0.643035  |

Cartesian coordinates of : L5

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.270638  | -0.954396 | 0.000249  |
| 1  | 0.908053  | -0.046205 | -0.029394 |
| 1  | 3.128055  | -0.378472 | 0.007451  |
| 1  | 2.316352  | -1.555643 | 0.820450  |
| 1  | 2.341188  | -1.572332 | -0.805652 |
| 7  | -4.874780 | 0.655026  | 0.023451  |
| 1  | -5.039916 | 1.215032  | -0.808728 |
| 1  | -4.993671 | 1.278041  | 0.817836  |
| 1  | -5.636802 | -0.016665 | 0.071102  |
| 7  | -2.270637 | -0.954396 | 0.000291  |
| 1  | -2.341185 | -1.572358 | -0.805591 |
| 1  | -2.316354 | -1.555616 | 0.820511  |
| 1  | -3.128055 | -0.378472 | 0.007471  |
| 7  | 0.000000  | 0.571604  | -0.048977 |
| 1  | -0.908053 | -0.046205 | -0.029378 |
| 1  | 0.000007  | 1.197180  | 0.755821  |
| 1  | -0.000008 | 1.145252  | -0.891573 |
| 7  | 4.874780  | 0.655027  | 0.023470  |
| 1  | 5.636791  | -0.016651 | 0.071483  |
| 1  | 4.993529  | 1.278306  | 0.817668  |
| 1  | 5.040070  | 1.214753  | -0.808867 |

Cartesian coordinates of : BC5\_2

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.623304 | -2.216940 | 0.149693  |
| 1  | -1.490562 | -1.674256 | -0.166435 |
| 1  | -0.853123 | -2.847689 | 0.915699  |
| 1  | -0.240386 | -2.763166 | -0.619903 |
| 1  | 0.089234  | -1.408446 | 0.476917  |
| 7  | 3.578723  | 0.178048  | -0.524670 |
| 1  | 4.183893  | -0.602801 | -0.284118 |
| 1  | 4.049253  | 1.015179  | -0.190418 |
| 1  | 3.577335  | 0.237066  | -1.539514 |
| 7  | -1.206556 | 2.447826  | 0.105780  |
| 1  | -2.063292 | 2.850769  | -0.268945 |
| 1  | -1.134287 | 2.801737  | 1.057285  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.451316 | 2.884920  | -0.417985 |
| 7 | -2.622151 | -0.420293 | -0.549946 |
| 1 | -2.164568 | 0.472494  | -0.343752 |
| 1 | -2.904216 | -0.399300 | -1.526964 |
| 1 | -3.479196 | -0.456025 | -0.003264 |
| 7 | 0.850281  | -0.101032 | 0.840443  |
| 1 | 1.048711  | -0.012838 | 1.834718  |
| 1 | 0.244673  | 0.681874  | 0.584031  |
| 1 | 1.748898  | 0.007221  | 0.343552  |

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Cartesian coordinates of : C5

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.888370  | 1.482815  | 0.380067  |
| 1  | 1.914372  | 1.777504  | 1.355357  |
| 1  | 2.167622  | 0.408587  | 0.297733  |
| 1  | 0.893273  | 1.616165  | -0.013947 |
| 1  | 2.546234  | 2.059121  | -0.143368 |
| 7  | -0.675737 | 1.751483  | -0.671479 |
| 1  | -0.676163 | 1.553075  | -1.669787 |
| 1  | -1.350061 | 1.107579  | -0.243337 |
| 1  | -1.059051 | 2.688930  | -0.570400 |
| 7  | -0.471084 | -2.014505 | -0.397309 |
| 1  | -0.688453 | -2.842824 | 0.150932  |
| 1  | -0.637007 | -2.264372 | -1.368652 |
| 1  | -1.156698 | -1.302977 | -0.147742 |
| 7  | 2.404347  | -1.153233 | 0.134702  |
| 1  | 2.770033  | -1.616113 | 0.963706  |
| 1  | 1.471907  | -1.549483 | -0.062337 |
| 1  | 3.019765  | -1.409749 | -0.633902 |
| 7  | -3.015100 | -0.045770 | 0.553601  |
| 1  | -3.577993 | -0.604018 | -0.084684 |
| 1  | -2.989545 | -0.557970 | 1.432500  |
| 1  | -3.563804 | 0.791014  | 0.740853  |

-----

Cartesian coordinates of : BC5\_3

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.726919 | -1.099336 | 0.031928  |
| 1  | -1.697420 | -1.445172 | 0.000295  |
| 1  | -2.634952 | -0.013620 | 0.029397  |
| 1  | -3.247632 | -1.424646 | -0.781144 |
| 1  | -3.196872 | -1.425216 | 0.875118  |
| 7  | 1.099713  | 1.451159  | -0.034529 |
| 1  | 1.184706  | 2.080515  | 0.761192  |
| 1  | 1.941830  | 0.860948  | -0.012583 |
| 1  | 1.194039  | 2.036707  | -0.861985 |
| 7  | -2.096676 | 1.555310  | 0.013279  |
| 1  | -2.396141 | 2.090923  | -0.798217 |
| 1  | -1.071132 | 1.511582  | -0.006469 |
| 1  | -2.364328 | 2.097274  | 0.831629  |
| 7  | -0.032508 | -1.571440 | -0.051519 |
| 1  | 0.377575  | -2.055957 | 0.743442  |
| 1  | 0.325626  | -2.031323 | -0.885223 |
| 1  | 0.342355  | -0.617015 | -0.048461 |
| 7  | 3.647412  | -0.353220 | 0.040472  |
| 1  | 4.389664  | 0.313616  | -0.156678 |
| 1  | 3.861422  | -0.753406 | 0.950079  |
| 1  | 3.754099  | -1.102529 | -0.637802 |

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Cartesian coordinates of the protonated ammonia hexamer

Cartesian coordinates of : BL6\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.831950  | 0.000579  | 0.011596  |
| 1  | 0.873878  | 0.866575  | 0.589896  |
| 1  | 0.879341  | -0.834711 | 0.633017  |
| 1  | -0.071653 | -0.016535 | -0.542715 |
| 1  | 1.640534  | -0.013514 | -0.646152 |
| 7  | -1.573254 | -0.048426 | -1.528544 |
| 1  | -1.622523 | -0.879877 | -2.112792 |
| 1  | -2.439090 | -0.031281 | -0.973774 |
| 1  | -1.624103 | 0.743568  | -2.165112 |
| 7  | 0.972227  | 2.473600  | 1.645899  |
| 1  | 0.194060  | 2.555573  | 2.295274  |
| 1  | 1.819671  | 2.526901  | 2.205442  |
| 1  | 0.955066  | 3.312134  | 1.070845  |
| 7  | 3.123269  | -0.039979 | -1.874179 |
| 1  | 3.142772  | -0.887194 | -2.436339 |
| 1  | 4.024392  | 0.013835  | -1.405986 |
| 1  | 3.093927  | 0.737315  | -2.529267 |
| 7  | -4.319574 | -0.000863 | -0.054840 |
| 1  | -4.524701 | 0.851275  | 0.459321  |
| 1  | -4.499823 | -0.773308 | 0.580290  |
| 1  | -5.015731 | -0.066356 | -0.792770 |
| 7  | 0.987356  | -2.385864 | 1.768881  |
| 1  | 0.962024  | -3.252807 | 1.237970  |
| 1  | 1.841292  | -2.412291 | 2.320406  |
| 1  | 0.216841  | -2.432623 | 2.430762  |

-----

Cartesian coordinates of : BC6\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.211229  | 0.000000  | 1.884449  |
| 1  | 1.998908  | 0.000001  | 1.233676  |
| 1  | 1.314358  | 0.814465  | 2.483818  |
| 1  | -0.355115 | 0.000000  | 0.834112  |
| 1  | 1.314359  | -0.814464 | 2.483819  |
| 7  | -2.710344 | -2.405403 | -0.000971 |
| 1  | -2.177028 | -3.271240 | -0.001859 |
| 1  | -3.319984 | -2.445513 | 0.812039  |
| 1  | -3.316771 | -2.441904 | -0.816554 |
| 7  | 3.919224  | 0.000000  | -0.014945 |
| 1  | 4.284160  | 0.813741  | 0.474983  |
| 1  | 4.375635  | 0.000007  | -0.924731 |
| 1  | 4.284158  | -0.813751 | 0.474969  |
| 7  | 1.195402  | 0.000000  | -1.878270 |
| 1  | 1.999961  | 0.000001  | -1.247360 |
| 1  | 1.285279  | -0.814377 | -2.480074 |
| 1  | 1.285278  | 0.814378  | -2.480074 |
| 7  | -2.710345 | 2.405403  | -0.000971 |
| 1  | -3.319985 | 2.445513  | 0.812039  |
| 1  | -2.177028 | 3.271239  | -0.001859 |
| 1  | -3.316771 | 2.441903  | -0.816554 |
| 7  | -0.994475 | 0.000000  | 0.006312  |
| 1  | -1.593300 | 0.854150  | 0.004148  |
| 1  | -0.347646 | 0.000000  | -0.817907 |
| 1  | -1.593300 | -0.854150 | 0.004148  |

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Cartesian coordinates of : BL6\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

```

-----
7      2.258234      0.468323      -1.099467
1      0.857218      -0.154312      -0.276206
1      2.973586      0.832076      -0.454067
1      2.714811      -0.238554      -1.671359
1      2.022935      1.230640      -1.730954
7      0.099393      -3.451436      0.422960
1      0.914821      -3.780194      0.934340
1      -0.711917      -3.839183      0.898300
1      0.135823      -3.896688      -0.490764
7      4.485066      1.605097      0.728975
1      5.209506      1.961796      0.111276
1      4.934308      0.924630      1.335619
1      4.205500      2.381544      1.322091
7      -0.005867      -0.527831      0.235963
1      -0.014996      -0.148660      1.181287
1      -0.900079      -0.220156      -0.266747
1      0.033169      -1.572387      0.295298
7      -2.353922      0.292769      -1.072989
1      -2.166342      0.979594      -1.799838
1      -3.035976      0.722232      -0.431868
1      -2.832748      -0.478215      -1.532895
7      -4.485625      1.608067      0.748510
1      -4.185624      2.455727      1.222130
1      -4.876894      1.000282      1.462920
1      -5.258061      1.874911      0.143773
-----

```

Cartesian coordinates of : BL6\_3

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-----
Atomic number (AN) and Cartesian coordinates

```

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.142463  | -0.836773 | 0.714768  |
| 1  | 0.783658  | -0.296229 | 0.048733  |
| 1  | 0.657204  | -1.031096 | 1.572195  |
| 1  | -0.721846 | -0.255307 | 0.960079  |
| 1  | -0.142438 | -1.748708 | 0.286425  |
| 7  | -2.113307 | 0.691763  | 1.418737  |
| 1  | -1.852064 | 1.514260  | 1.957967  |
| 1  | -2.661605 | 1.030936  | 0.616190  |
| 1  | -2.756520 | 0.165895  | 2.006277  |
| 7  | 1.855678  | 0.587155  | -0.997118 |
| 1  | 1.477049  | 1.497873  | -1.246734 |
| 1  | 2.774756  | 0.757957  | -0.564788 |
| 1  | 2.032287  | 0.105118  | -1.875449 |
| 7  | -0.629482 | -3.418779 | -0.436527 |
| 1  | -1.141604 | -3.995013 | 0.227010  |
| 1  | 0.174319  | -3.967875 | -0.731366 |
| 1  | -1.227099 | -3.323555 | -1.253876 |
| 7  | -3.902576 | 1.809697  | -0.857084 |
| 1  | -3.796985 | 1.441277  | -1.798110 |
| 1  | -3.792193 | 2.817730  | -0.927294 |
| 1  | -4.869687 | 1.645714  | -0.590059 |
| 7  | 4.652128  | 1.154320  | 0.206043  |
| 1  | 5.199335  | 1.606421  | -0.521803 |
| 1  | 4.650348  | 1.789068  | 0.999808  |
| 1  | 5.178746  | 0.333848  | 0.493061  |

Cartesian coordinates of : BL6\_4

```

-----
Atomic number (AN) and Cartesian coordinates

```

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.026153 | -0.554460 | 0.281346  |
| 1  | -0.070071 | -0.214833 | 1.240602  |
| 1  | 0.741491  | -0.018476 | -0.238267 |
| 1  | 0.195276  | -1.577602 | 0.299373  |
| 1  | -0.976403 | -0.391610 | -0.185322 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -4.495706 | 1.604015  | 0.716605  |
| 1 | -4.741701 | 1.222704  | 1.625896  |
| 1 | -5.359589 | 1.655022  | 0.183221  |
| 1 | -4.198907 | 2.562884  | 0.875411  |
| 7 | 1.982316  | 0.871907  | -1.073543 |
| 1 | 1.638759  | 1.760208  | -1.431588 |
| 1 | 2.341816  | 0.365165  | -1.879189 |
| 1 | 2.792582  | 1.090196  | -0.476686 |
| 7 | 4.467371  | 1.617455  | 0.620685  |
| 1 | 5.037315  | 0.831052  | 0.919833  |
| 1 | 5.059900  | 2.192632  | 0.027754  |
| 1 | 4.273450  | 2.167431  | 1.452981  |
| 7 | -2.524076 | -0.123737 | -0.931657 |
| 1 | -2.440026 | 0.340332  | -1.833167 |
| 1 | -3.021145 | -0.993517 | -1.109274 |
| 1 | -3.148775 | 0.459192  | -0.356764 |
| 7 | 0.581111  | -3.421766 | 0.356171  |
| 1 | -0.069963 | -3.939973 | 0.940969  |
| 1 | 0.541755  | -3.850319 | -0.565329 |
| 1 | 1.510199  | -3.614376 | 0.722296  |

-----

Cartesian coordinates of : BC6\_2

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.842081  | 1.867359  | 0.216824  |
| 1  | 2.608915  | 1.211452  | 0.052748  |
| 1  | 2.118359  | 2.468609  | 0.988709  |
| 1  | 1.773407  | 2.463296  | -0.603975 |
| 1  | 0.341425  | 0.868369  | 0.529970  |
| 7  | -0.319793 | 0.058490  | 0.659308  |
| 1  | 0.275963  | -0.791465 | 0.479588  |
| 1  | -1.154388 | 0.112982  | -0.015571 |
| 1  | -0.661918 | 0.042962  | 1.618052  |
| 7  | 1.695420  | -1.884058 | 0.101548  |
| 1  | 1.915776  | -2.558553 | 0.829682  |
| 1  | 1.585331  | -2.413832 | -0.759116 |
| 1  | 2.514864  | -1.283644 | -0.015085 |
| 7  | -5.239957 | -0.137603 | 0.351591  |
| 1  | -5.368531 | -1.025008 | 0.829858  |
| 1  | -5.954588 | -0.094364 | -0.370190 |
| 1  | -5.467219 | 0.589464  | 1.024305  |
| 7  | -2.513981 | 0.205487  | -1.063462 |
| 1  | -2.493357 | -0.505238 | -1.791155 |
| 1  | -2.570663 | 1.100292  | -1.544403 |
| 1  | -3.404459 | 0.085411  | -0.559055 |
| 7  | 4.450878  | -0.100942 | -0.245594 |
| 1  | 4.792589  | -0.931714 | -0.724064 |
| 1  | 4.827218  | 0.686202  | -0.769647 |
| 1  | 4.918736  | -0.086351 | 0.657849  |

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Cartesian coordinates of : BC6\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.512123 | -0.189533 | -0.723520 |
| 1  | -1.257919 | 0.842224  | -0.553856 |
| 1  | -1.480885 | -0.382957 | -1.722972 |
| 1  | -0.785674 | -0.784657 | -0.231469 |
| 1  | -2.475786 | -0.402005 | -0.368249 |
| 7  | 3.504523  | -1.323658 | -0.522572 |
| 1  | 4.254681  | -1.187982 | 0.151452  |
| 1  | 3.782433  | -0.823416 | -1.363775 |
| 1  | 3.529331  | -2.310982 | -0.768197 |
| 7  | 2.241644  | 1.578065  | 0.563953  |
| 1  | 2.883943  | 2.229755  | 0.120810  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 2.431509  | 1.624521  | 1.561372  |
| 1 | 2.499722  | 0.643513  | 0.250008  |
| 7 | -0.637687 | 2.394978  | -0.205889 |
| 1 | 0.334101  | 2.219745  | 0.084055  |
| 1 | -0.612524 | 3.040579  | -0.991141 |
| 1 | -1.102033 | 2.885506  | 0.554166  |
| 7 | -4.214448 | -0.765073 | 0.210963  |
| 1 | -4.501984 | -1.722947 | 0.025337  |
| 1 | -4.900093 | -0.167347 | -0.244531 |
| 1 | -4.328966 | -0.620584 | 1.211225  |
| 7 | 0.521413  | -1.642711 | 0.642978  |
| 1 | 0.562740  | -1.326858 | 1.609154  |
| 1 | 0.398494  | -2.651798 | 0.678563  |
| 1 | 1.445660  | -1.468773 | 0.236645  |

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Cartesian coordinates of : BC6\_4

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 3.937929  | -1.139733 | 0.588411  |
| 1  | 2.333853  | -0.651831 | -0.238298 |
| 1  | 4.036434  | -0.736511 | 1.516912  |
| 1  | 4.025398  | -2.146669 | 0.702813  |
| 1  | 4.752497  | -0.839865 | 0.058035  |
| 7  | 1.445726  | -0.392637 | -0.730838 |
| 1  | 0.570748  | -0.656393 | -0.157155 |
| 1  | 1.362069  | 0.653578  | -0.857470 |
| 1  | 1.419180  | -0.852878 | -1.638560 |
| 7  | -2.132256 | 2.471110  | 0.649740  |
| 1  | -2.255783 | 2.408476  | 1.657695  |
| 1  | -2.981754 | 2.096735  | 0.233454  |
| 1  | -2.135193 | 3.465826  | 0.434028  |
| 7  | -0.899428 | -0.679320 | 0.694476  |
| 1  | -1.261475 | 0.274863  | 0.662657  |
| 1  | -1.612557 | -1.303256 | 0.293638  |
| 1  | -0.806424 | -0.929239 | 1.675841  |
| 7  | 0.766413  | 2.357528  | -0.823857 |
| 1  | 0.621254  | 2.768068  | -1.742721 |
| 1  | 1.369075  | 2.998595  | -0.314312 |
| 1  | -0.140117 | 2.349439  | -0.347662 |
| 7  | -3.033021 | -2.644482 | -0.424447 |
| 1  | -2.686273 | -3.599257 | -0.387543 |
| 1  | -3.868246 | -2.620605 | 0.154437  |
| 1  | -3.340219 | -2.486340 | -1.380188 |

-----

Cartesian coordinates of : BL6\_5

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.300563  | -0.095496 | -0.592302 |
| 1  | 0.302654  | -0.094716 | -0.097682 |
| 1  | 1.172181  | -0.226794 | -1.594230 |
| 1  | 1.791502  | 0.814772  | -0.438134 |
| 1  | 1.889828  | -0.879211 | -0.228990 |
| 7  | 2.699324  | 2.459523  | -0.192341 |
| 1  | 2.351473  | 3.190713  | -0.807718 |
| 1  | 2.600399  | 2.811739  | 0.756551  |
| 1  | 3.698296  | 2.387971  | -0.369401 |
| 7  | -1.136436 | -0.108196 | 0.587047  |
| 1  | -1.659019 | 0.762107  | 0.422147  |
| 1  | -1.716815 | -0.883697 | 0.240901  |
| 1  | -1.076886 | -0.220942 | 1.596774  |
| 7  | -2.841448 | 2.488176  | 0.181359  |
| 1  | -3.761267 | 2.262897  | 0.550779  |
| 1  | -2.521604 | 3.308253  | 0.689069  |
| 1  | -2.981452 | 2.779384  | -0.782065 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -2.974949 | -2.445363 | -0.395834 |
| 1 | -3.864203 | -2.323744 | 0.081376  |
| 1 | -2.655659 | -3.383874 | -0.172528 |
| 1 | -3.179021 | -2.438132 | -1.391321 |
| 7 | 2.962674  | -2.307774 | 0.403513  |
| 1 | 2.462800  | -3.193453 | 0.403023  |
| 1 | 3.279457  | -2.158453 | 1.358345  |
| 1 | 3.799240  | -2.450907 | -0.156995 |

-----

Cartesian coordinates of : BC6\_5

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.064753 | 0.086921  | -0.849828 |
| 1  | -1.214988 | 0.708424  | -0.701323 |
| 1  | -1.725815 | -0.881963 | -0.570974 |
| 1  | -2.884915 | 0.396460  | -0.270341 |
| 1  | -2.328662 | 0.091004  | -1.833367 |
| 7  | 2.288651  | -1.220521 | 0.355216  |
| 1  | 2.640020  | -1.944541 | -0.268121 |
| 1  | 2.965163  | -0.448591 | 0.295024  |
| 1  | 2.378000  | -1.597416 | 1.296474  |
| 7  | -0.732830 | -2.254113 | -0.062895 |
| 1  | -1.018724 | -2.682659 | 0.813737  |
| 1  | 0.214636  | -1.886534 | 0.070902  |
| 1  | -0.672964 | -3.006127 | -0.744812 |
| 7  | 0.415096  | 1.311405  | -0.355017 |
| 1  | 0.869320  | 1.781105  | -1.134210 |
| 1  | 0.470191  | 1.948288  | 0.435711  |
| 1  | 0.988647  | 0.494366  | -0.123532 |
| 7  | -4.367676 | 0.939070  | 0.694118  |
| 1  | -5.156954 | 0.308430  | 0.574563  |
| 1  | -4.694474 | 1.861922  | 0.417568  |
| 1  | -4.188671 | 0.986752  | 1.694261  |
| 7  | 4.369266  | 1.109680  | 0.161167  |
| 1  | 4.586526  | 1.408457  | -0.785667 |
| 1  | 5.222664  | 0.701897  | 0.534519  |
| 1  | 4.196716  | 1.953631  | 0.700257  |

-----

Cartesian coordinates of : BL6\_6

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.891782  | -0.000423 | -0.471712 |
| 1  | 0.957526  | 0.019415  | 0.091039  |
| 1  | 1.670421  | 0.017433  | -1.466101 |
| 1  | 2.476116  | 0.840571  | -0.243526 |
| 1  | 2.427402  | -0.878255 | -0.263700 |
| 7  | 3.505345  | 2.352629  | 0.136755  |
| 1  | 3.058203  | 3.213256  | -0.169988 |
| 1  | 3.679585  | 2.460493  | 1.133007  |
| 1  | 4.417819  | 2.329524  | -0.312168 |
| 7  | -0.500855 | 0.050457  | 0.884031  |
| 1  | -0.615267 | 0.863872  | 1.484493  |
| 1  | -1.279135 | 0.072566  | 0.198881  |
| 1  | -0.654358 | -0.761737 | 1.477369  |
| 7  | -5.504787 | -0.069320 | 0.435891  |
| 1  | -6.245417 | -0.078393 | -0.259692 |
| 1  | -5.623237 | -0.906739 | 0.998564  |
| 1  | -5.688225 | 0.721732  | 1.046297  |
| 7  | -2.767372 | 0.124280  | -1.094779 |
| 1  | -3.642070 | 0.052805  | -0.561778 |
| 1  | -2.780024 | -0.632337 | -1.773551 |
| 1  | -2.826480 | 0.985786  | -1.631342 |
| 7  | 3.371312  | -2.453897 | 0.080088  |
| 1  | 2.806548  | -3.285290 | -0.076475 |

```

1      3.695999      -2.505753      1.042595
1      4.196614      -2.555024      -0.505848
-----

```

Cartesian coordinates of : Cs6\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.438450 | 1.591806  | 0.000000  |
| 1  | -1.662178 | 0.983716  | 0.834706  |
| 1  | -1.998455 | 2.441409  | 0.000000  |
| 1  | -0.403069 | 1.822319  | 0.000001  |
| 1  | -1.662177 | 0.983718  | -0.834707 |
| 7  | 1.364600  | 2.057688  | 0.000004  |
| 1  | 1.877010  | 1.171348  | 0.000005  |
| 1  | 1.677788  | 2.581226  | 0.814049  |
| 1  | 1.677791  | 2.581226  | -0.814039 |
| 7  | 0.335795  | -2.028987 | -0.000003 |
| 1  | 0.496453  | -2.625221 | 0.808949  |
| 1  | 0.496461  | -2.625211 | -0.808961 |
| 1  | 1.079105  | -1.329628 | 0.000005  |
| 7  | -1.882525 | -0.486451 | 1.850619  |
| 1  | -1.371043 | -1.186181 | 1.309858  |
| 1  | -1.480549 | -0.461474 | 2.783861  |
| 1  | -2.839581 | -0.812658 | 1.955767  |
| 7  | -1.882524 | -0.486443 | -1.850619 |
| 1  | -1.480550 | -0.461462 | -2.783861 |
| 1  | -2.839580 | -0.812651 | -1.955767 |
| 1  | -1.371041 | -1.186175 | -1.309862 |
| 7  | 3.323492  | -0.512051 | 0.000000  |
| 1  | 3.496586  | -1.097945 | 0.813727  |
| 1  | 4.067727  | 0.182632  | 0.000009  |
| 1  | 3.496585  | -1.097922 | -0.813745 |

-----

Cartesian coordinates of : Cs6\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.656913 | -0.951004 | -1.941298 |
| 1  | -1.375072 | -0.521923 | -1.357028 |
| 1  | -1.086661 | -1.731267 | -2.431322 |
| 1  | -0.392350 | -0.271752 | -2.649919 |
| 1  | 0.744301  | -1.392468 | -0.833300 |
| 7  | 1.374512  | -1.504893 | -0.000003 |
| 1  | 0.744294  | -1.392485 | 0.833289  |
| 1  | 2.107938  | -0.722227 | 0.000005  |
| 1  | 1.817866  | -2.420849 | -0.000011 |
| 7  | -0.656950 | -0.951054 | 1.941275  |
| 1  | -0.392405 | -0.271834 | 2.649933  |
| 1  | -1.375093 | -0.521947 | 1.357005  |
| 1  | -1.086711 | -1.731338 | 2.431252  |
| 7  | 0.124537  | 1.997892  | 0.000036  |
| 1  | -0.689422 | 1.384624  | 0.000018  |
| 1  | 0.037585  | 2.603352  | -0.812421 |
| 1  | 0.037605  | 2.603276  | 0.812552  |
| 7  | 3.002992  | 0.733916  | 0.000004  |
| 1  | 3.575280  | 0.930930  | -0.816293 |
| 1  | 3.575276  | 0.930938  | 0.816302  |
| 1  | 2.207470  | 1.378695  | 0.000000  |
| 7  | -2.961462 | 0.551277  | -0.000015 |
| 1  | -3.207611 | 1.118771  | 0.809254  |
| 1  | -3.207593 | 1.118793  | -0.809274 |
| 1  | -3.621715 | -0.224232 | -0.000033 |

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Cartesian coordinates of : BC6\_6

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.198402 | 1.543318  | -0.653245 |
| 1  | -2.874108 | -0.349950 | -0.251269 |
| 1  | -2.886243 | 2.190808  | -0.277273 |
| 1  | -1.297441 | 1.795353  | -0.248167 |
| 1  | -2.144569 | 1.732832  | -1.650428 |
| 7  | 1.020372  | -0.202479 | -0.454718 |
| 1  | 0.808555  | 0.712192  | -0.044981 |
| 1  | 0.832173  | -0.122672 | -1.451978 |
| 1  | 2.033215  | -0.365326 | -0.357864 |
| 7  | -0.502033 | -2.156415 | 0.619608  |
| 1  | -0.363607 | -2.219432 | 1.626893  |
| 1  | -0.272513 | -3.060836 | 0.210650  |
| 1  | 0.152961  | -1.361101 | 0.190205  |
| 7  | -3.041257 | -1.332580 | 0.009232  |
| 1  | -1.540624 | -1.904461 | 0.404957  |
| 1  | -3.721895 | -1.342233 | 0.764877  |
| 1  | -3.483292 | -1.793203 | -0.782510 |
| 7  | 4.066344  | -0.743528 | -0.264680 |
| 1  | 4.318352  | -1.596615 | -0.756837 |
| 1  | 4.582316  | 0.007731  | -0.715189 |
| 1  | 4.447211  | -0.830802 | 0.673659  |
| 7  | 0.565237  | 2.771796  | 0.740470  |
| 1  | 1.523395  | 2.757036  | 1.082973  |
| 1  | -0.007368 | 3.051974  | 1.533375  |
| 1  | 0.521645  | 3.537927  | 0.072236  |

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Cartesian coordinates of : BC6\_7

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.012008  | 1.998213  | 0.906880  |
| 1  | -0.857441 | 1.329120  | 0.869435  |
| 1  | 0.873194  | 1.303947  | 0.865003  |
| 1  | 0.015922  | 2.636658  | 0.113929  |
| 1  | 0.018612  | 2.543738  | 1.766511  |
| 7  | 0.009456  | -2.653819 | 0.361954  |
| 1  | -0.346247 | -3.114817 | 1.196345  |
| 1  | -0.607949 | -2.926509 | -0.399429 |
| 1  | 0.903052  | -3.097666 | 0.161124  |
| 7  | 1.876744  | 0.055259  | 0.779195  |
| 1  | 2.574803  | 0.128261  | 0.025201  |
| 1  | 1.303549  | -0.775118 | 0.608886  |
| 1  | 2.390879  | -0.110089 | 1.641437  |
| 7  | -1.887175 | 0.066996  | 0.786689  |
| 1  | -2.404310 | -0.095010 | 1.647622  |
| 1  | -2.582154 | 0.134767  | 0.029612  |
| 1  | -1.312223 | -0.761938 | 0.622003  |
| 7  | 4.079560  | 0.319211  | -1.374776 |
| 1  | 4.619038  | 1.169232  | -1.234194 |
| 1  | 4.735284  | -0.452923 | -1.289465 |
| 1  | 3.772515  | 0.329646  | -2.343551 |
| 7  | -4.084031 | 0.316682  | -1.375997 |
| 1  | -3.779519 | 0.334803  | -2.345449 |
| 1  | -4.737176 | -0.458011 | -1.294182 |
| 1  | -4.625760 | 1.164115  | -1.228458 |

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Cartesian coordinates of : L6

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -3.403762 | -1.024356 | -0.074103 |
| 1  | -2.063810 | -0.035309 | 0.041365  |

-----

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -3.454310 | -1.696799 | 0.688257  |
| 1 | -4.287672 | -0.492269 | -0.058440 |
| 1 | -3.407873 | -1.571498 | -0.932311 |
| 7 | -6.090438 | 0.467052  | -0.038522 |
| 1 | -6.279986 | 0.990821  | 0.811715  |
| 1 | -6.232675 | 1.111117  | -0.811915 |
| 1 | -6.822916 | -0.234366 | -0.111785 |
| 7 | -1.195898 | 0.617315  | 0.117062  |
| 1 | -1.258151 | 1.160291  | 0.977313  |
| 1 | -0.242086 | 0.037331  | 0.112429  |
| 1 | -1.197540 | 1.270730  | -0.665120 |
| 7 | 3.434612  | 1.140292  | -0.064812 |
| 1 | 3.502466  | 1.796796  | 0.708625  |
| 1 | 4.299707  | 0.586537  | -0.053822 |
| 1 | 3.461347  | 1.700264  | -0.913069 |
| 7 | 1.134785  | -0.748274 | 0.103338  |
| 1 | 1.934906  | -0.086043 | 0.045185  |
| 1 | 1.221752  | -1.386636 | -0.684763 |
| 1 | 1.276972  | -1.310681 | 0.939829  |
| 7 | 6.135890  | -0.450434 | -0.039666 |
| 1 | 6.251062  | -1.096165 | -0.815546 |
| 1 | 6.890128  | 0.226941  | -0.110903 |
| 1 | 6.302357  | -0.982227 | 0.809870  |

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Cartesian coordinates of : DC6\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.384299  | -2.228036 | 0.192624  |
| 1  | 0.513434  | -1.738762 | -0.247131 |
| 1  | 2.194606  | -1.477777 | 0.264260  |
| 1  | 1.154328  | -2.585285 | 1.118533  |
| 1  | 1.678300  | -3.011692 | -0.388310 |
| 7  | 1.539233  | 2.213199  | -0.156052 |
| 1  | 1.684031  | 2.616725  | -1.078063 |
| 1  | 0.529364  | 2.123808  | -0.024035 |
| 1  | 1.862384  | 2.911304  | 0.509186  |
| 7  | 3.243101  | -0.262646 | 0.312531  |
| 1  | 3.719154  | -0.156997 | 1.205561  |
| 1  | 2.703478  | 0.602965  | 0.143509  |
| 1  | 3.971465  | -0.312634 | -0.396215 |
| 7  | -0.703028 | -0.846744 | -0.927530 |
| 1  | -0.800196 | -1.010731 | -1.927056 |
| 1  | -1.632909 | -0.967120 | -0.512560 |
| 1  | -0.487329 | 0.143928  | -0.805703 |
| 7  | -1.665378 | 1.930046  | 0.210345  |
| 1  | -2.275586 | 1.122063  | 0.330363  |
| 1  | -1.719727 | 2.470353  | 1.070239  |
| 1  | -2.082289 | 2.507899  | -0.515373 |
| 7  | -3.649337 | -0.858432 | 0.352454  |
| 1  | -4.351280 | -0.358030 | -0.188089 |
| 1  | -3.851156 | -0.664990 | 1.330651  |
| 1  | -3.852293 | -1.846730 | 0.219624  |

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Cartesian coordinates of : DC6\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.642654 | -1.859914 | 0.018271  |
| 1  | -2.090089 | -0.993094 | -0.284605 |
| 1  | -2.139181 | -2.168152 | 0.850996  |
| 1  | -1.839553 | -2.556667 | -0.696215 |
| 1  | 0.411075  | -1.973894 | 0.220270  |
| 7  | 1.426275  | -2.122868 | 0.321599  |
| 1  | 1.612483  | -2.227901 | 1.316768  |
| 1  | 2.319057  | -0.886787 | -0.359276 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.632318  | -3.027217 | -0.097808 |
| 7 | -0.818492 | 1.042763  | 1.220055  |
| 1 | -1.145372 | 1.541324  | 2.043488  |
| 1 | -1.595943 | 1.007646  | 0.558958  |
| 1 | -0.648565 | 0.081124  | 1.503233  |
| 7 | 1.701671  | 2.225312  | 0.044010  |
| 1 | 0.806483  | 1.911999  | 0.456689  |
| 1 | 1.487028  | 2.899556  | -0.686929 |
| 1 | 2.210131  | 2.734064  | 0.763714  |
| 7 | 2.884364  | -0.062981 | -0.790199 |
| 1 | 2.866470  | -0.131551 | -1.806776 |
| 1 | 3.855783  | -0.117119 | -0.486747 |
| 1 | 2.440836  | 0.901178  | -0.470530 |
| 7 | -3.404730 | 0.802747  | -0.804391 |
| 1 | -4.221173 | 0.627059  | -0.223405 |
| 1 | -3.376233 | 1.808677  | -0.954132 |
| 1 | -3.610592 | 0.394345  | -1.713110 |

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Cartesian coordinates of : BC6\_8

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.270430  | 2.162539  | 0.327342  |
| 1  | 2.837044  | 0.966309  | -0.081329 |
| 1  | 1.346104  | 2.988787  | -0.260478 |
| 1  | 0.346508  | 1.762660  | 0.160819  |
| 1  | 1.284161  | 2.495693  | 1.287703  |
| 7  | -0.342132 | -1.191293 | 0.916056  |
| 1  | -0.738020 | -0.341864 | 0.490902  |
| 1  | -0.160186 | -0.972743 | 1.893368  |
| 1  | -1.086254 | -1.885714 | 0.915520  |
| 7  | 1.969709  | -1.986343 | -0.366620 |
| 1  | 1.771511  | -2.269482 | -1.325209 |
| 1  | 2.395679  | -2.776064 | 0.116495  |
| 1  | 1.046216  | -1.703465 | 0.130775  |
| 7  | 3.521489  | 0.226320  | -0.306671 |
| 1  | 2.660627  | -1.118960 | -0.363962 |
| 1  | 3.977252  | 0.479678  | -1.180222 |
| 1  | 4.243130  | 0.241094  | 0.410267  |
| 7  | -4.451371 | -0.484037 | -0.252195 |
| 1  | -4.762208 | -0.751154 | 0.677843  |
| 1  | -5.148513 | 0.163373  | -0.611084 |
| 1  | -4.512648 | -1.317620 | -0.830172 |
| 7  | -1.830943 | 1.240361  | -0.324111 |
| 1  | -2.668420 | 0.644152  | -0.314992 |
| 1  | -1.716820 | 1.552796  | -1.285802 |
| 1  | -2.075441 | 2.069700  | 0.212958  |

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Cartesian coordinates of : BC6\_9

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 3.311985  | -0.000055 | -0.383627 |
| 1  | 2.662305  | -0.858323 | -0.200277 |
| 1  | 2.662353  | 0.858240  | -0.200270 |
| 1  | 4.107563  | -0.000077 | 0.252517  |
| 1  | 3.657774  | -0.000058 | -1.341704 |
| 7  | -1.067094 | 0.000015  | 0.713877  |
| 1  | -1.548725 | 0.824362  | 0.338387  |
| 1  | -1.548760 | -0.824314 | 0.338392  |
| 1  | -1.250548 | 0.000021  | 1.715118  |
| 7  | 1.405501  | 1.866521  | 0.157250  |
| 1  | 1.554526  | 2.454411  | 0.974011  |
| 1  | 0.602188  | 1.257066  | 0.358554  |
| 1  | 1.124720  | 2.487113  | -0.598281 |
| 7  | 1.405436  | -1.866553 | 0.157232  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.124639  | -2.487133 | -0.598304 |
| 1 | 1.554443  | -2.454452 | 0.973990  |
| 1 | 0.602140  | -1.257076 | 0.358538  |
| 7 | -2.464569 | 2.663007  | -0.315377 |
| 1 | -3.428002 | 2.506504  | -0.030481 |
| 1 | -2.486656 | 2.824541  | -1.318470 |
| 1 | -2.180492 | 3.538893  | 0.114619  |
| 7 | -2.464678 | -2.662937 | -0.315364 |
| 1 | -2.486866 | -2.824418 | -1.318463 |
| 1 | -3.428078 | -2.506423 | -0.030366 |
| 1 | -2.180582 | -3.538854 | 0.114558  |

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Cartesian coordinates of : BC6\_10

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.060776  | 0.043164  | -0.789308 |
| 1  | 1.583111  | -0.837057 | -0.987016 |
| 1  | 3.005420  | -0.155693 | -0.346281 |
| 1  | 2.206037  | 0.528421  | -1.674328 |
| 1  | 1.391527  | 0.668261  | -0.114971 |
| 7  | 0.408695  | 1.483178  | 0.738701  |
| 1  | 0.270948  | 1.112164  | 1.677077  |
| 1  | -0.523272 | 1.497313  | 0.275482  |
| 1  | 0.702656  | 2.451156  | 0.856142  |
| 7  | -1.022968 | -1.654147 | -0.220398 |
| 1  | -0.361795 | -1.882585 | 0.511277  |
| 1  | -0.830439 | -2.189690 | -1.057962 |
| 1  | -1.046951 | -0.657124 | -0.410988 |
| 7  | -3.968413 | -0.816266 | 0.510288  |
| 1  | -3.239947 | -1.524619 | 0.426523  |
| 1  | -4.758565 | -1.112975 | -0.054816 |
| 1  | -4.287892 | -0.808595 | 1.474295  |
| 7  | -2.254460 | 1.437070  | -0.597132 |
| 1  | -2.341218 | 1.356332  | -1.607965 |
| 1  | -2.611868 | 2.363373  | -0.371439 |
| 1  | -2.925828 | 0.764618  | -0.192794 |
| 7  | 4.614397  | -0.481650 | 0.364567  |
| 1  | 5.164174  | -1.125764 | -0.200118 |
| 1  | 5.173525  | 0.363895  | 0.455900  |
| 1  | 4.564197  | -0.890880 | 1.294954  |

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Cartesian coordinates of the protonated ammonia heptamer

Cartesian coordinates of : BC7\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.155616 | -0.587604 | 0.159982  |
| 1  | -0.963300 | -0.057656 | 0.588700  |
| 1  | 0.626832  | -0.676917 | 0.843745  |
| 1  | -0.471411 | -1.527809 | -0.153608 |
| 1  | 0.256461  | -0.054154 | -0.636337 |
| 7  | -1.075234 | -3.282395 | -0.704773 |
| 1  | -0.790702 | -4.011074 | -0.055222 |
| 1  | -2.089115 | -3.329918 | -0.764238 |
| 1  | -0.720084 | -3.555178 | -1.617534 |
| 7  | -2.335670 | 0.838636  | 1.357359  |
| 1  | -2.716820 | 0.335799  | 2.155229  |
| 1  | -2.044049 | 1.746344  | 1.711803  |
| 1  | -3.121217 | 1.013106  | 0.717564  |
| 7  | 1.498500  | 0.907864  | -1.719401 |
| 1  | 2.383167  | 0.942064  | -1.208787 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.220362  | 1.867897  | -1.904047 |
| 1 | 1.688759  | 0.482584  | -2.622735 |
| 7 | -4.802063 | 1.464443  | -0.450835 |
| 1 | -5.086391 | 2.422149  | -0.263724 |
| 1 | -5.594148 | 0.876332  | -0.206852 |
| 1 | -4.682684 | 1.388937  | -1.456937 |
| 7 | 4.458265  | 1.139091  | -0.264787 |
| 1 | 4.703749  | 1.741168  | 0.517789  |
| 1 | 5.126570  | 0.372010  | -0.254379 |
| 1 | 4.668275  | 1.677225  | -1.102668 |
| 7 | 2.344363  | -0.516385 | 1.665869  |
| 1 | 2.932017  | 0.005771  | 1.013710  |
| 1 | 2.336144  | -0.003586 | 2.543329  |
| 1 | 2.809772  | -1.400653 | 1.851304  |

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Cartesian coordinates of : BL7\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.003333 | -0.725435 | -0.014289 |
| 1  | -0.009257 | -0.803678 | -1.050804 |
| 1  | -0.436148 | -1.576636 | 0.396970  |
| 1  | 0.991448  | -0.643941 | 0.327671  |
| 1  | -0.550403 | 0.126462  | 0.281770  |
| 7  | 2.704452  | -0.546604 | 0.955376  |
| 1  | 3.251075  | -1.366235 | 0.702245  |
| 1  | 3.226429  | 0.269622  | 0.612357  |
| 1  | 2.727880  | -0.497163 | 1.971125  |
| 7  | -0.003214 | -0.971840 | -2.991741 |
| 1  | 0.813925  | -1.471754 | -3.332411 |
| 1  | -0.814996 | -1.470551 | -3.346536 |
| 1  | 0.001260  | -0.064838 | -3.450997 |
| 7  | -1.459661 | 1.612541  | 0.831484  |
| 1  | -1.466335 | 1.688240  | 1.845829  |
| 1  | -2.441392 | 1.646875  | 0.529577  |
| 1  | -1.021624 | 2.464551  | 0.489830  |
| 7  | 4.465943  | 1.868101  | 0.041206  |
| 1  | 4.212149  | 2.752431  | 0.472554  |
| 1  | 4.524388  | 2.038517  | -0.958704 |
| 1  | 5.409227  | 1.654543  | 0.353918  |
| 7  | -1.211772 | -3.177963 | 1.190575  |
| 1  | -1.100854 | -3.190453 | 2.201199  |
| 1  | -2.208885 | -3.259438 | 1.009639  |
| 1  | -0.785050 | -4.033230 | 0.843907  |
| 7  | -4.466035 | 1.909958  | 0.024104  |
| 1  | -5.078241 | 1.148693  | 0.303422  |
| 1  | -4.798885 | 2.740282  | 0.506762  |
| 1  | -4.630374 | 2.066402  | -0.966327 |

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Cartesian coordinates of : BC7\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.450202 | -0.065770 | 0.005180  |
| 1  | -1.095546 | 0.623800  | 0.719742  |
| 1  | -1.686793 | -0.972676 | 0.456710  |
| 1  | -2.288650 | 0.314915  | -0.480763 |
| 1  | -0.658096 | -0.177279 | -0.670981 |
| 7  | -3.849372 | 1.024656  | -1.366515 |
| 1  | -4.599358 | 1.235248  | -0.712911 |
| 1  | -3.650608 | 1.889325  | -1.863260 |
| 1  | -4.237263 | 0.382195  | -2.052593 |
| 7  | -0.103163 | 1.800675  | 1.696158  |
| 1  | -0.090423 | 1.615200  | 2.695649  |
| 1  | 0.862055  | 1.709736  | 1.357787  |
| 1  | -0.369704 | 2.776144  | 1.591324  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 0.953880  | 0.097632  | -1.587627 |
| 1 | 1.730877  | -0.488650 | -1.275806 |
| 1 | 1.212241  | 1.051810  | -1.344814 |
| 1 | 0.922623  | 0.043819  | -2.602142 |
| 7 | -2.190803 | -2.634198 | 1.309449  |
| 1 | -1.418414 | -3.065120 | 1.810828  |
| 1 | -2.936170 | -2.502776 | 1.988552  |
| 1 | -2.525485 | -3.327588 | 0.645329  |
| 7 | 3.668663  | -1.529874 | -0.743113 |
| 1 | 4.018525  | -1.881152 | 0.145080  |
| 1 | 3.378576  | -2.349953 | -1.270723 |
| 1 | 4.473011  | -1.149284 | -1.236190 |
| 7 | 2.862276  | 1.359164  | 0.700325  |
| 1 | 3.069883  | 0.452136  | 0.281744  |
| 1 | 3.339111  | 1.388661  | 1.598019  |
| 1 | 3.310653  | 2.065489  | 0.122416  |

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Cartesian coordinates of : BC7\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.757514 | -0.013865 | -0.064931 |
| 1  | -0.910842 | -0.093899 | -0.679951 |
| 1  | -1.362572 | 0.086283  | 0.901814  |
| 1  | -2.319236 | 0.825659  | -0.318654 |
| 1  | -2.345811 | -0.870504 | -0.135212 |
| 7  | 2.872740  | 0.185425  | 1.213574  |
| 1  | 3.128782  | -0.520207 | 1.900696  |
| 1  | 3.534049  | 0.073453  | 0.434879  |
| 1  | 3.092573  | 1.082668  | 1.640421  |
| 7  | -0.168772 | 0.242420  | 2.318940  |
| 1  | -0.238259 | 1.113886  | 2.837381  |
| 1  | 0.766412  | 0.209382  | 1.903338  |
| 1  | -0.221446 | -0.505717 | 3.004947  |
| 7  | 0.846090  | -0.181494 | -1.278506 |
| 1  | 1.102372  | -1.066612 | -1.707575 |
| 1  | 1.105460  | 0.544299  | -1.941157 |
| 1  | 1.445782  | -0.063881 | -0.456611 |
| 7  | 4.930604  | -0.157649 | -1.129787 |
| 1  | 4.893202  | 0.541326  | -1.866219 |
| 1  | 5.843353  | -0.065426 | -0.691852 |
| 1  | 4.921320  | -1.064855 | -1.587214 |
| 7  | -3.446297 | -2.443850 | -0.259607 |
| 1  | -3.897665 | -2.532166 | -1.166459 |
| 1  | -4.189599 | -2.451786 | 0.434170  |
| 1  | -2.913748 | -3.298572 | -0.119524 |
| 7  | -3.373503 | 2.370583  | -0.771580 |
| 1  | -4.288400 | 2.356674  | -0.328032 |
| 1  | -2.929049 | 3.238828  | -0.484437 |
| 1  | -3.540119 | 2.450175  | -1.771466 |

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Cartesian coordinates of : BC7\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.337911  | 0.065101  | 0.051224  |
| 1  | 2.072299  | 0.242998  | -0.663634 |
| 1  | 1.678800  | -0.634138 | 0.741162  |
| 1  | 1.073891  | 0.955694  | 0.532627  |
| 1  | 0.440258  | -0.257642 | -0.408242 |
| 7  | 0.090190  | 2.429315  | 1.169456  |
| 1  | 0.052996  | 2.499490  | 2.182830  |
| 1  | 0.418988  | 3.329445  | 0.830471  |
| 1  | -0.871366 | 2.314127  | 0.838705  |
| 7  | 3.447905  | 0.573341  | -1.987470 |
| 1  | 4.325676  | 0.871749  | -1.569930 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.658392  | -0.253197 | -2.540986 |
| 1 | 3.181501  | 1.300412  | -2.646423 |
| 7 | -1.247555 | -0.366305 | -1.019449 |
| 1 | -1.763583 | -1.221298 | -0.781620 |
| 1 | -1.319665 | -0.252820 | -2.027279 |
| 1 | -1.737926 | 0.422807  | -0.597409 |
| 7 | 2.361077  | -1.909771 | 2.032775  |
| 1 | 2.630314  | -2.791034 | 1.603133  |
| 1 | 3.183117  | -1.564265 | 2.521382  |
| 1 | 1.674905  | -2.135551 | 2.748190  |
| 7 | -2.867747 | -3.003877 | -0.480190 |
| 1 | -3.143683 | -3.195856 | 0.478613  |
| 1 | -3.722992 | -2.980283 | -1.028705 |
| 1 | -2.342965 | -3.813524 | -0.799086 |
| 7 | -3.022336 | 2.228218  | 0.227386  |
| 1 | -3.321075 | 2.435102  | -0.722666 |
| 1 | -3.188532 | 3.077600  | 0.762497  |
| 1 | -3.675464 | 1.538026  | 0.590257  |

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Cartesian coordinates of : BDC7\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 4.212485  | 0.000460  | 0.892118  |
| 1  | 2.403763  | -0.000580 | 0.253407  |
| 1  | 4.469940  | 0.881853  | 1.328920  |
| 1  | 4.382769  | -0.724190 | 1.584771  |
| 1  | 4.881306  | -0.155119 | 0.142082  |
| 7  | 1.428659  | -0.000951 | -0.110884 |
| 1  | 0.707583  | -0.000055 | 0.646735  |
| 1  | 1.220788  | 0.854185  | -0.674022 |
| 1  | 1.220698  | -0.857348 | -0.672117 |
| 7  | -2.514980 | 2.838566  | 0.286701  |
| 1  | -2.326694 | 3.383813  | 1.124691  |
| 1  | -3.398431 | 2.361394  | 0.450228  |
| 1  | -2.701433 | 3.513810  | -0.451461 |
| 7  | -1.055041 | 0.000785  | 1.294073  |
| 1  | -1.507065 | 0.828039  | 0.902704  |
| 1  | -1.508111 | -0.825927 | 0.902771  |
| 1  | -1.225886 | 0.000947  | 2.295296  |
| 7  | 0.309747  | 2.369456  | -1.343581 |
| 1  | 0.081624  | 2.320963  | -2.332826 |
| 1  | 0.799769  | 3.248663  | -1.202096 |
| 1  | -0.571917 | 2.426860  | -0.829498 |
| 7  | -2.519438 | -2.834527 | 0.285652  |
| 1  | -2.333863 | -3.380551 | 1.123741  |
| 1  | -2.706345 | -3.509032 | -0.453071 |
| 1  | -3.401983 | -2.355256 | 0.447926  |
| 7  | 0.310283  | -2.373978 | -1.338553 |
| 1  | 0.799543  | -3.252778 | -1.191973 |
| 1  | -0.572643 | -2.428687 | -0.826350 |
| 1  | 0.084585  | -2.329691 | -2.328547 |

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Cartesian coordinates of : BL7\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X        | Y         | Z         |
|----|----------|-----------|-----------|
| 7  | 1.779169 | -0.064146 | -0.000002 |
| 1  | 0.819213 | -0.524125 | -0.000038 |
| 1  | 2.307971 | -0.349456 | 0.850038  |
| 1  | 2.308052 | -0.349488 | -0.849981 |
| 1  | 1.647219 | 0.969538  | -0.000028 |
| 7  | 1.221528 | 2.840818  | -0.000072 |
| 1  | 1.566039 | 3.342116  | 0.814413  |
| 1  | 0.210012 | 2.944666  | -0.000006 |
| 1  | 1.565925 | 3.342045  | -0.814648 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -3.027735 | 0.925642  | 0.000030  |
| 1 | -3.090175 | 1.531507  | -0.813728 |
| 1 | -3.878748 | 0.351870  | 0.000014  |
| 1 | -3.090153 | 1.531429  | 0.813848  |
| 7 | -0.813606 | -1.202347 | -0.000099 |
| 1 | -1.523757 | -0.453803 | -0.000055 |
| 1 | -1.003338 | -1.783956 | -0.812665 |
| 1 | -1.003353 | -1.784066 | 0.812384  |
| 7 | 3.292213  | -0.880175 | 2.428643  |
| 1 | 2.828339  | -0.593221 | 3.286725  |
| 1 | 4.226838  | -0.481043 | 2.460192  |
| 1 | 3.408293  | -1.888547 | 2.488866  |
| 7 | -5.695688 | -0.748382 | -0.000021 |
| 1 | -5.813380 | -1.342626 | 0.815358  |
| 1 | -5.813402 | -1.342523 | -0.815473 |
| 1 | -6.474086 | -0.095378 | 0.000031  |
| 7 | 3.292440  | -0.880250 | -2.428481 |
| 1 | 4.227090  | -0.481167 | -2.459920 |
| 1 | 3.408473  | -1.888627 | -2.488697 |
| 1 | 2.828680  | -0.593265 | -3.286614 |

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Cartesian coordinates of : BDC7\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.169077  | -0.101521 | -0.021215 |
| 1  | 0.778299  | -0.767156 | -0.747595 |
| 1  | 2.169387  | -0.317744 | 0.179121  |
| 1  | 1.070105  | 0.875550  | -0.343198 |
| 1  | 0.576957  | -0.255059 | 0.834456  |
| 7  | -2.145104 | 1.829365  | 0.555333  |
| 1  | -2.847738 | 2.189819  | -0.085430 |
| 1  | -1.235871 | 2.020905  | 0.139412  |
| 1  | -2.214952 | 2.397121  | 1.396267  |
| 7  | -2.942521 | -1.232514 | -0.372156 |
| 1  | -3.552830 | -1.181835 | -1.184006 |
| 1  | -3.448453 | -1.780484 | 0.318836  |
| 1  | -2.852776 | -0.285008 | -0.003708 |
| 7  | -0.197569 | -1.947634 | -1.672460 |
| 1  | -1.133251 | -1.862962 | -1.256656 |
| 1  | -0.291544 | -1.778682 | -2.670411 |
| 1  | 0.097004  | -2.915568 | -1.573401 |
| 7  | 3.987696  | -0.772638 | 0.565964  |
| 1  | 4.033453  | -1.518545 | 1.255742  |
| 1  | 4.535733  | -0.002777 | 0.941194  |
| 1  | 4.487098  | -1.109184 | -0.253460 |
| 7  | -0.792150 | -0.690754 | 1.967338  |
| 1  | -1.165762 | -1.582548 | 1.651322  |
| 1  | -0.680719 | -0.745776 | 2.975433  |
| 1  | -1.499035 | 0.014985  | 1.758963  |
| 7  | 0.943540  | 2.794432  | -1.002086 |
| 1  | 0.864423  | 3.541556  | -0.315936 |
| 1  | 1.866869  | 2.898903  | -1.417829 |
| 1  | 0.282821  | 3.013339  | -1.744146 |

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Cartesian coordinates of : BDC7\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.533911  | 1.377561  | -2.825970 |
| 1  | -0.319627 | 1.754688  | -3.230756 |
| 1  | 0.827989  | 0.618799  | -3.435769 |
| 1  | 1.237278  | 2.106712  | -2.913903 |
| 1  | 0.232071  | 0.817590  | -1.022010 |
| 7  | -3.255344 | -1.123067 | 0.252964  |
| 1  | -2.372954 | -1.605015 | 0.090862  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -3.722178 | -1.595351 | 1.022136  |
| 1 | -3.836378 | -1.264324 | -0.568414 |
| 7 | 0.025748  | 0.528724  | -0.040644 |
| 1 | -0.828345 | 1.057769  | 0.314403  |
| 1 | -0.163386 | -0.493834 | -0.020436 |
| 1 | 0.841372  | 0.741154  | 0.558798  |
| 7 | 2.283906  | 1.418475  | 1.819615  |
| 1 | 1.810712  | 2.246739  | 2.175396  |
| 1 | 3.191345  | 1.741665  | 1.491519  |
| 1 | 2.464514  | 0.832910  | 2.632124  |
| 7 | -2.352714 | 1.734311  | 0.856475  |
| 1 | -2.765787 | 2.481166  | 0.304821  |
| 1 | -2.914990 | 0.886095  | 0.716460  |
| 1 | -2.441382 | 2.009501  | 1.830758  |
| 7 | 2.801812  | -1.481242 | 0.018261  |
| 1 | 3.356609  | -2.109948 | 0.593273  |
| 1 | 3.278466  | -1.416908 | -0.876944 |
| 1 | 2.848633  | -0.562079 | 0.451641  |
| 7 | -0.150954 | -2.440924 | -0.064769 |
| 1 | -0.421530 | -2.980765 | -0.883138 |
| 1 | 0.871153  | -2.350054 | -0.087092 |
| 1 | -0.378141 | -3.013372 | 0.744748  |

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Cartesian coordinates of : BC7\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.517732  | -2.501975 | 0.231289  |
| 1  | -0.340408 | -0.985793 | 0.336998  |
| 1  | 0.218475  | -3.114209 | -0.523131 |
| 1  | 1.490666  | -2.228001 | 0.041607  |
| 1  | 0.517393  | -3.066749 | 1.076661  |
| 7  | 3.376898  | -1.411032 | -0.275946 |
| 1  | 3.684240  | -1.479739 | -1.242224 |
| 1  | 3.498028  | -0.441151 | 0.012612  |
| 1  | 4.027267  | -1.969179 | 0.270774  |
| 7  | -0.722526 | 0.010783  | 0.355709  |
| 1  | 0.012672  | 0.638489  | -0.065107 |
| 1  | -1.639176 | 0.079402  | -0.185413 |
| 1  | -0.887328 | 0.289071  | 1.321071  |
| 7  | -5.664924 | 0.450908  | 0.769262  |
| 1  | -6.477361 | 0.458896  | 0.158322  |
| 1  | -5.801423 | -0.317365 | 1.420288  |
| 1  | -5.707494 | 1.306254  | 1.316324  |
| 7  | -3.165179 | 0.185151  | -1.050089 |
| 1  | -3.970971 | 0.274124  | -0.415848 |
| 1  | -3.334619 | -0.638870 | -1.622138 |
| 1  | -3.203064 | 0.980575  | -1.683088 |
| 7  | 1.390593  | 1.555687  | -0.834892 |
| 1  | 2.250679  | 1.517013  | -0.280927 |
| 1  | 1.605988  | 1.144350  | -1.739920 |
| 1  | 1.191858  | 2.537958  | -1.007597 |
| 7  | 4.180831  | 1.649348  | 0.790630  |
| 1  | 4.381073  | 1.226443  | 1.693935  |
| 1  | 5.035042  | 1.573764  | 0.243049  |
| 1  | 4.054479  | 2.642628  | 0.972016  |

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Cartesian coordinates of : BTC7\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X        | Y         | Z         |
|----|----------|-----------|-----------|
| 7  | 1.711210 | -0.837199 | 0.556399  |
| 1  | 1.514777 | -1.175804 | -0.442317 |
| 1  | 1.795524 | -1.646483 | 1.168902  |
| 1  | 2.604966 | -0.296519 | 0.595671  |
| 1  | 0.882483 | -0.241976 | 0.881168  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 4.273151  | 0.596580  | 0.684895  |
| 1 | 5.039377  | -0.005094 | 0.392597  |
| 1 | 4.306796  | 1.415864  | 0.083501  |
| 1 | 4.502409  | 0.918287  | 1.622029  |
| 7 | 0.955886  | -1.639114 | -2.000236 |
| 1 | 1.419461  | -1.208068 | -2.795403 |
| 1 | 0.913696  | -2.635993 | -2.194301 |
| 1 | -0.008503 | -1.281167 | -1.961813 |
| 7 | -0.537970 | 0.646854  | 1.351128  |
| 1 | -0.785212 | 1.351696  | 0.651153  |
| 1 | -0.454912 | 1.129810  | 2.242202  |
| 1 | -1.335346 | 0.009075  | 1.429237  |
| 7 | -1.770276 | -0.392572 | -1.381215 |
| 1 | -2.137565 | -0.761150 | -0.504875 |
| 1 | -2.485986 | -0.530395 | -2.089445 |
| 1 | -1.659644 | 0.612607  | -1.253216 |
| 7 | -1.467840 | 2.897104  | -0.806191 |
| 1 | -1.180814 | 3.030651  | -1.772840 |
| 1 | -2.472426 | 3.054780  | -0.780646 |
| 1 | -1.050536 | 3.663695  | -0.283628 |
| 7 | -3.064537 | -1.372260 | 1.571619  |
| 1 | -3.954663 | -0.920975 | 1.374786  |
| 1 | -3.010578 | -1.455530 | 2.584133  |
| 1 | -3.140675 | -2.323072 | 1.218312  |

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Cartesian coordinates of : BL7\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.483905  | 0.185111  | -1.029269 |
| 1  | 0.981018  | 0.198364  | -0.087760 |
| 1  | 2.377159  | 0.636743  | -1.934415 |
| 1  | 3.258632  | 0.663595  | -0.550347 |
| 1  | 2.800950  | -0.761867 | -1.222551 |
| 7  | 4.893344  | 1.601712  | 0.330325  |
| 1  | 4.768267  | 2.597035  | 0.492151  |
| 1  | 5.179881  | 1.197253  | 1.217406  |
| 1  | 5.686655  | 1.509210  | -0.298344 |
| 7  | 0.088980  | 0.214428  | 0.491477  |
| 1  | -0.718263 | 0.605900  | -0.079512 |
| 1  | -0.142676 | -0.762903 | 0.839007  |
| 1  | 0.237947  | 0.818253  | 1.297931  |
| 7  | -1.323752 | -4.545248 | -0.614704 |
| 1  | -0.954251 | -5.434358 | -0.288950 |
| 1  | -2.332528 | -4.655792 | -0.669015 |
| 1  | -0.993082 | -4.426178 | -1.567912 |
| 7  | -0.513671 | -2.383308 | 1.474080  |
| 1  | -0.777005 | -3.055249 | 0.741010  |
| 1  | -1.280404 | -2.368007 | 2.142442  |
| 1  | 0.279320  | -2.787723 | 1.966566  |
| 7  | -2.071217 | 1.280688  | -1.007455 |
| 1  | -2.538849 | 2.058077  | -0.522190 |
| 1  | -1.779940 | 1.636509  | -1.914736 |
| 1  | -2.785683 | 0.581311  | -1.194601 |
| 7  | -3.555603 | 3.639559  | 0.369456  |
| 1  | -3.950868 | 3.425379  | 1.280722  |
| 1  | -2.994793 | 4.478864  | 0.486126  |
| 1  | -4.335399 | 3.894991  | -0.230398 |

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Cartesian coordinates of : DC7\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.068535 | -2.034254 | -0.619126 |
| 1  | -0.014237 | -2.154038 | 0.439329  |
| 1  | -0.951040 | -1.507370 | -0.866886 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.776805  | -1.498231 | -0.957630 |
| 1 | -0.087097 | -2.948570 | -1.067200 |
| 7 | 2.236452  | -0.604847 | -1.548549 |
| 1 | 3.060299  | -1.200443 | -1.509626 |
| 1 | 2.146962  | -0.306432 | -2.516802 |
| 1 | 2.450078  | 0.231919  | -0.997351 |
| 7 | -2.859943 | 2.213496  | 0.087731  |
| 1 | -2.288394 | 3.032965  | -0.102465 |
| 1 | -3.748507 | 2.379420  | -0.379724 |
| 1 | -3.062393 | 2.226441  | 1.084501  |
| 7 | 0.048442  | 0.864280  | 1.084077  |
| 1 | 0.052064  | 1.570070  | 1.816233  |
| 1 | 0.873779  | 1.034564  | 0.511235  |
| 1 | -0.775200 | 1.044552  | 0.511951  |
| 7 | 3.042909  | 1.997792  | 0.098363  |
| 1 | 3.273679  | 1.891900  | 1.083387  |
| 1 | 2.583816  | 2.900419  | 0.003833  |
| 1 | 3.931954  | 2.086062  | -0.388911 |
| 7 | 0.065556  | -2.045807 | 2.169107  |
| 1 | -0.730084 | -2.365178 | 2.713974  |
| 1 | 0.901888  | -2.376213 | 2.641573  |
| 1 | 0.072349  | -1.022077 | 2.170167  |
| 7 | -2.473131 | -0.628761 | -1.283131 |
| 1 | -2.550455 | 0.285029  | -0.826087 |
| 1 | -2.571219 | -0.469104 | -2.282877 |
| 1 | -3.287303 | -1.168980 | -0.999931 |

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Cartesian coordinates of : BC7\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -3.332291 | 2.966836  | 0.026859  |
| 1  | -1.901885 | 1.790812  | -0.381359 |
| 1  | -3.388580 | 3.754364  | -0.614189 |
| 1  | -4.235864 | 2.501550  | -0.009330 |
| 1  | -3.249946 | 3.362082  | 0.960208  |
| 7  | -1.120831 | 1.142058  | -0.626911 |
| 1  | -1.108848 | 0.999624  | -1.634575 |
| 1  | -0.190170 | 1.526178  | -0.310249 |
| 1  | -1.211776 | 0.178760  | -0.113888 |
| 7  | 4.015701  | 0.553495  | -1.005262 |
| 1  | 4.160243  | 1.407313  | -1.539524 |
| 1  | 4.073284  | -0.207005 | -1.678333 |
| 1  | 4.828521  | 0.461978  | -0.400328 |
| 7  | 2.133159  | -1.352401 | 1.010625  |
| 1  | 2.671516  | -0.774801 | 0.365025  |
| 1  | 2.573686  | -1.271251 | 1.923423  |
| 1  | 2.261800  | -2.318832 | 0.721882  |
| 7  | 1.410101  | 1.751521  | 0.512719  |
| 1  | 1.351255  | 1.162162  | 1.340761  |
| 1  | 1.651817  | 2.688240  | 0.824482  |
| 1  | 2.200198  | 1.394765  | -0.030545 |
| 7  | -1.043928 | -1.216543 | 0.735001  |
| 1  | -1.373461 | -2.058426 | 0.246344  |
| 1  | -0.037198 | -1.317009 | 0.904898  |
| 1  | -1.502059 | -1.208671 | 1.642993  |
| 7  | -2.155963 | -3.800359 | -0.637803 |
| 1  | -1.999368 | -4.585964 | -0.012266 |
| 1  | -3.160639 | -3.738727 | -0.777646 |
| 1  | -1.754167 | -4.059390 | -1.534379 |

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Cartesian coordinates of : BDC7\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z        |
|----|-----------|-----------|----------|
| 7  | -2.051942 | -0.412072 | 0.740318 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.141646 | -0.688227 | 0.249113  |
| 1 | -2.019340 | 0.655200  | 0.788311  |
| 1 | -2.894848 | -0.745498 | 0.216679  |
| 1 | -2.068863 | -0.798113 | 1.682138  |
| 7 | -4.439182 | -1.340569 | -0.673817 |
| 1 | -4.472314 | -1.026425 | -1.640546 |
| 1 | -4.515692 | -2.354442 | -0.699097 |
| 1 | -5.289972 | -0.999816 | -0.232568 |
| 7 | 0.402683  | -0.713722 | -0.542066 |
| 1 | 0.757268  | 0.241855  | -0.468447 |
| 1 | 1.126596  | -1.326743 | -0.157590 |
| 1 | 0.343883  | -0.924196 | -1.535579 |
| 7 | 3.570283  | 0.377272  | -0.343367 |
| 1 | 4.306958  | 0.659950  | 0.297190  |
| 1 | 3.271266  | -0.557566 | -0.070294 |
| 1 | 3.999210  | 0.299518  | -1.261455 |
| 7 | 2.700388  | -2.739256 | 0.539803  |
| 1 | 3.137536  | -2.624838 | 1.451135  |
| 1 | 3.429846  | -3.068616 | -0.088208 |
| 1 | 2.047471  | -3.513173 | 0.637763  |
| 7 | 1.333401  | 2.555570  | -0.386555 |
| 1 | 1.295562  | 2.933378  | -1.330359 |
| 1 | 1.582369  | 3.337823  | 0.214770  |
| 1 | 2.129797  | 1.908097  | -0.360928 |
| 7 | -1.600523 | 2.342734  | 0.705959  |
| 1 | -0.643149 | 2.386078  | 0.332476  |
| 1 | -2.191239 | 2.895503  | 0.089923  |
| 1 | -1.596463 | 2.820560  | 1.603645  |

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Cartesian coordinates of : BC7\_7

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -5.287087 | -1.350297 | -0.000914 |
| 1  | -5.017721 | -2.214114 | -0.463015 |
| 1  | -6.158527 | -1.053604 | -0.432379 |
| 1  | -5.511521 | -1.591899 | 0.960440  |
| 1  | -4.010489 | 0.316445  | -0.164863 |
| 7  | -3.395195 | 1.136590  | -0.237375 |
| 1  | -3.564651 | 1.534404  | -1.158649 |
| 1  | -1.348665 | 1.929741  | -0.032278 |
| 1  | -3.757111 | 1.814933  | 0.429491  |
| 7  | -1.307880 | -1.288314 | 0.235531  |
| 1  | -1.371116 | -1.883008 | -0.586561 |
| 1  | -1.688644 | -1.825262 | 1.010257  |
| 1  | -1.939088 | -0.496290 | 0.082456  |
| 7  | 1.143694  | 0.080704  | 0.649683  |
| 1  | 0.335401  | -0.588252 | 0.525710  |
| 1  | 1.474059  | 0.046683  | 1.611930  |
| 1  | 1.954831  | -0.144132 | -0.010943 |
| 7  | -0.427518 | 2.367691  | 0.064391  |
| 1  | -0.505469 | 3.081902  | 0.783687  |
| 1  | -0.230731 | 2.854902  | -0.805827 |
| 1  | 0.725309  | 1.030095  | 0.449558  |
| 7  | 3.299623  | -0.507225 | -1.051562 |
| 1  | 4.200531  | -0.466355 | -0.554396 |
| 1  | 3.367935  | 0.140747  | -1.832807 |
| 1  | 3.234187  | -1.436415 | -1.460592 |
| 7  | 6.055960  | -0.413459 | 0.359609  |
| 1  | 6.759754  | -0.630948 | -0.340886 |
| 1  | 6.174930  | -1.091594 | 1.107037  |
| 1  | 6.305612  | 0.492193  | 0.747096  |

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Cartesian coordinates of : BC7\_8

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

```

-----
7      2.276807      -0.122080      0.740886
1      2.174274      -0.328335      1.732788
1      3.279941      -0.251519      0.469715
1      1.640167      -0.766477      0.180521
1      1.950986      0.883807      0.551884
7      1.199586      2.368032      0.135813
1      1.047232      3.011856      0.907894
1      0.275800      2.085958      -0.221801
1      1.663572      2.900764      -0.595373
7      -4.950686      0.264101      0.399593
1      -5.186760      0.673070      -0.500316
1      -5.718944      -0.355782      0.643226
1      -4.967536      1.019414      1.079277
7      -2.463608      -1.649684      0.353205
1      -3.266940      -1.010889      0.393813
1      -2.311719      -1.976895      1.304437
1      -2.776709      -2.460960      -0.175412
7      -1.520002      1.281824      -0.832808
1      -1.640033      1.270781      -1.842285
1      -2.242075      1.898820      -0.469892
1      -1.746981      0.346317      -0.493605
7      5.094373      -0.473824      0.036011
1      5.454169      -1.387887      0.299696
1      5.268847      -0.373913      -0.960949
1      5.685199      0.211686      0.500362
7      0.474818      -1.654487      -0.797129
1      0.436488      -1.260437      -1.734302
1      -0.472627      -1.581307      -0.407598
1      0.674638      -2.645247      -0.911070
-----

```

Cartesian coordinates of : BC7\_9

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Atomic number (AN) and Cartesian coordinates

```

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.086068 | -0.019929 | -0.766801 |
| 1  | -1.991635 | 0.038239  | -1.779190 |
| 1  | -1.657739 | -0.946792 | -0.429036 |
| 1  | -1.553900 | 0.790958  | -0.324732 |
| 1  | -3.102608 | 0.028012  | -0.521767 |
| 7  | -0.845893 | -2.337492 | 0.151025  |
| 1  | -0.637653 | -3.042638 | -0.551287 |
| 1  | -1.318772 | -2.820743 | 0.910527  |
| 1  | 0.051826  | -1.988743 | 0.519138  |
| 7  | 1.696598  | -1.012471 | 1.213008  |
| 1  | 2.457289  | -0.968020 | 0.534242  |
| 1  | 2.064035  | -1.453659 | 2.051518  |
| 1  | 1.480015  | -0.048315 | 1.452127  |
| 7  | 2.463531  | 1.892347  | -0.000227 |
| 1  | 2.627652  | 2.597203  | -0.714732 |
| 1  | 2.976288  | 2.202421  | 0.821653  |
| 1  | 2.915600  | 1.034494  | -0.321061 |
| 7  | -4.944071 | 0.095296  | -0.127196 |
| 1  | -5.461078 | 0.698081  | -0.762618 |
| 1  | -5.380046 | -0.821839 | -0.184056 |
| 1  | -5.128012 | 0.443021  | 0.810587  |
| 7  | -0.623724 | 2.095733  | 0.407952  |
| 1  | -0.865151 | 3.009323  | 0.030953  |
| 1  | -0.775668 | 2.158431  | 1.411901  |
| 1  | 0.388381  | 1.975565  | 0.265652  |
| 7  | 4.231789  | -0.743818 | -0.886817 |
| 1  | 5.052455  | -0.636503 | -0.295630 |
| 1  | 4.459689  | -0.298387 | -1.772363 |
| 1  | 4.153897  | -1.737775 | -1.088428 |

Cartesian coordinates of : DC7\_2

## Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 4.377918  | 0.399398  | -0.015646 |
| 1  | 4.452437  | 0.925586  | -0.883078 |
| 1  | 5.058851  | -0.353396 | -0.088113 |
| 1  | 4.719435  | 1.010802  | 0.722375  |
| 1  | 2.741445  | -1.037101 | 0.333922  |
| 7  | 2.091876  | -1.804543 | 0.528685  |
| 1  | 2.587594  | -2.669293 | 0.325932  |
| 1  | 0.539449  | -1.669611 | -0.408600 |
| 1  | 1.925965  | -1.802694 | 1.532119  |
| 7  | 1.521655  | 2.066493  | 0.507906  |
| 1  | 1.867865  | 2.962267  | 0.175106  |
| 1  | 1.389805  | 2.162464  | 1.510776  |
| 1  | 2.265003  | 1.384486  | 0.364565  |
| 7  | -0.952942 | 1.134578  | -1.108769 |
| 1  | -0.215621 | 1.584854  | -0.552931 |
| 1  | -1.836775 | 1.209646  | -0.604437 |
| 1  | -1.049856 | 1.647416  | -1.980338 |
| 7  | -0.355289 | -1.543240 | -0.953114 |
| 1  | -1.196989 | -1.819820 | -0.386164 |
| 1  | -0.317799 | -2.083635 | -1.814431 |
| 1  | -0.514678 | -0.497095 | -1.159702 |
| 7  | -3.936412 | 1.350578  | 0.436334  |
| 1  | -3.582002 | 2.191646  | 0.885821  |
| 1  | -4.397729 | 1.655289  | -0.417720 |
| 1  | -4.676862 | 1.005760  | 1.043441  |
| 7  | -2.798985 | -1.718819 | 0.511136  |
| 1  | -3.094388 | -0.739603 | 0.473397  |
| 1  | -3.540436 | -2.273429 | 0.091131  |
| 1  | -2.759460 | -1.985660 | 1.491202  |

Cartesian coordinates of : BL7\_4

## Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.312503  | -0.207981 | -0.979628 |
| 1  | -0.191937 | -0.543670 | -0.253517 |
| 1  | 1.276195  | 0.577128  | -1.625644 |
| 1  | 2.018268  | 0.029595  | -0.260814 |
| 1  | 1.685666  | -0.991785 | -1.510097 |
| 7  | 3.389375  | 0.496692  | 1.109722  |
| 1  | 3.560464  | -0.224065 | 1.805790  |
| 1  | 4.279182  | 0.649970  | 0.621878  |
| 1  | 3.192008  | 1.349017  | 1.627340  |
| 7  | -1.131445 | -0.744293 | 0.237216  |
| 1  | -1.932116 | -0.256103 | -0.272412 |
| 1  | -1.305233 | -1.774322 | 0.276626  |
| 1  | -1.083095 | -0.386380 | 1.189556  |
| 7  | -4.881093 | 2.533931  | 0.650317  |
| 1  | -5.276077 | 2.142759  | 1.501006  |
| 1  | -4.371129 | 3.369095  | 0.924592  |
| 1  | -5.666187 | 2.848143  | 0.086127  |
| 7  | -1.613644 | -3.643210 | 0.367381  |
| 1  | -1.707851 | -4.059481 | -0.555706 |
| 1  | -2.462083 | -3.878458 | 0.876400  |
| 1  | -0.855053 | -4.138490 | 0.829511  |
| 7  | -3.248792 | 0.559159  | -1.099989 |
| 1  | -3.765348 | 1.205478  | -0.487611 |
| 1  | -2.918865 | 1.107697  | -1.890723 |
| 1  | -3.932171 | -0.093593 | -1.476633 |
| 7  | 6.162791  | 0.990990  | -0.295891 |
| 1  | 6.159543  | 1.772918  | -0.944422 |
| 1  | 6.519319  | 0.188404  | -0.806496 |
| 1  | 6.848650  | 1.209136  | 0.421355  |

Cartesian coordinates of : BC7\_10

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.549136  | -1.407876 | -0.928541 |
| 1  | 0.600615  | -1.749528 | -0.602982 |
| 1  | 1.430882  | -0.333169 | -0.991916 |
| 1  | 2.308337  | -1.687466 | -0.266395 |
| 1  | 1.753895  | -1.789800 | -1.849751 |
| 7  | -2.317615 | 1.124897  | -0.122880 |
| 1  | -2.530678 | 1.672247  | -0.953899 |
| 1  | -3.186557 | 0.632783  | 0.120423  |
| 1  | -2.156804 | 1.798115  | 0.622959  |
| 7  | 0.854963  | 1.248742  | -1.022779 |
| 1  | 1.355590  | 1.919853  | -0.426749 |
| 1  | -0.113041 | 1.194129  | -0.696817 |
| 1  | 0.829291  | 1.651684  | -1.956382 |
| 7  | -1.117736 | -1.832555 | -0.104856 |
| 1  | -1.712931 | -2.376413 | -0.724328 |
| 1  | -1.272024 | -2.194459 | 0.832577  |
| 1  | -1.470041 | -0.869091 | -0.118290 |
| 7  | -4.989249 | -0.353711 | 0.591135  |
| 1  | -4.987388 | -0.896414 | 1.450134  |
| 1  | -5.681847 | 0.379937  | 0.715506  |
| 1  | -5.344980 | -0.964387 | -0.138995 |
| 7  | 2.386014  | 3.420125  | 0.620426  |
| 1  | 3.368992  | 3.458991  | 0.365476  |
| 1  | 2.351109  | 3.352401  | 1.633640  |
| 1  | 1.989745  | 4.324023  | 0.377437  |
| 7  | 3.705034  | -2.257044 | 0.868248  |
| 1  | 3.622339  | -1.871988 | 1.805730  |
| 1  | 3.730451  | -3.268301 | 0.973827  |
| 1  | 4.621213  | -1.981189 | 0.523519  |

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Cartesian coordinates of : BC7\_11

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.906020 | -1.879901 | 0.142435  |
| 1  | -1.405529 | -0.870657 | 0.550956  |
| 1  | -3.221362 | -2.490501 | 0.891543  |
| 1  | -3.660001 | -1.217368 | -0.049119 |
| 1  | -2.798966 | -2.464366 | -0.682346 |
| 7  | -5.486810 | 0.094502  | -0.484887 |
| 1  | -6.034419 | -0.346794 | 0.250538  |
| 1  | -5.900451 | 1.014705  | -0.619826 |
| 1  | -5.687079 | -0.423010 | -1.337840 |
| 7  | -0.766966 | -0.055925 | 0.725974  |
| 1  | -0.479125 | -0.049491 | 1.702575  |
| 1  | 0.114270  | -0.088645 | 0.096553  |
| 1  | -1.362495 | 0.787928  | 0.526386  |
| 7  | 3.916449  | 0.068548  | 1.034589  |
| 1  | 4.764386  | 0.052662  | 0.456515  |
| 1  | 3.954394  | 0.924604  | 1.581510  |
| 1  | 4.004147  | -0.696240 | 1.698534  |
| 7  | 1.531350  | -0.136699 | -0.808897 |
| 1  | 2.351355  | -0.066934 | -0.180088 |
| 1  | 1.608835  | 0.624299  | -1.479617 |
| 1  | 1.640940  | -0.996370 | -1.341803 |
| 7  | 6.576423  | 0.024716  | -0.645599 |
| 1  | 7.357380  | 0.107185  | -0.000804 |
| 1  | 6.719281  | -0.834214 | -1.168877 |
| 1  | 6.663113  | 0.789527  | -1.308571 |
| 7  | -2.776106 | 1.883079  | 0.094881  |
| 1  | -2.623091 | 2.438066  | -0.743052 |
| 1  | -3.584670 | 1.282613  | -0.082222 |
| 1  | -3.039150 | 2.534762  | 0.829583  |

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Cartesian coordinates of : BC7\_12

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.599860 | -0.101451 | 1.077932  |
| 1  | -1.604665 | -0.044709 | 2.094059  |
| 1  | -0.620302 | 0.228188  | 0.683818  |
| 1  | -1.669912 | -1.108616 | 0.780852  |
| 1  | -2.394850 | 0.459751  | 0.702837  |
| 7  | 1.647106  | -2.695452 | -1.264259 |
| 1  | 2.492094  | -2.619917 | -0.703371 |
| 1  | 1.561099  | -3.679419 | -1.508481 |
| 1  | 1.834145  | -2.207293 | -2.136594 |
| 7  | 1.185937  | 2.577379  | -2.207201 |
| 1  | 2.164278  | 2.596122  | -2.481542 |
| 1  | 0.965492  | 3.507273  | -1.862095 |
| 1  | 0.648896  | 2.448607  | -3.059915 |
| 7  | -3.893213 | 1.475823  | 0.094655  |
| 1  | -4.374677 | 1.956776  | 0.850277  |
| 1  | -3.625157 | 2.190545  | -0.576837 |
| 1  | -4.589337 | 0.894212  | -0.364722 |
| 7  | 0.850460  | 0.395635  | 0.051784  |
| 1  | 0.925300  | 1.099310  | -0.691752 |
| 1  | 1.083984  | -0.509673 | -0.356545 |
| 1  | 1.564767  | 0.609236  | 0.757910  |
| 7  | 3.007979  | 1.088739  | 2.248101  |
| 1  | 2.930169  | 2.069222  | 2.503631  |
| 1  | 3.951347  | 0.957182  | 1.894142  |
| 1  | 2.947204  | 0.558873  | 3.112916  |
| 7  | -1.290144 | -2.760223 | 0.081621  |
| 1  | -1.259076 | -3.508375 | 0.769177  |
| 1  | -1.930108 | -3.065292 | -0.646822 |
| 1  | -0.358541 | -2.695153 | -0.339366 |

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Cartesian coordinates of : TC7\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.188372  | -2.021639 | 0.000003  |
| 1  | 0.623325  | -1.693307 | 0.820146  |
| 1  | 0.623326  | -1.693307 | -0.820141 |
| 1  | 2.138912  | -1.511752 | 0.000002  |
| 1  | 1.304498  | -3.032000 | 0.000003  |
| 7  | 3.458105  | -0.455241 | -0.000003 |
| 1  | 4.063312  | -0.505269 | -0.815334 |
| 1  | 3.002378  | 0.466720  | -0.000006 |
| 1  | 4.063316  | -0.505263 | 0.815325  |
| 7  | -0.590573 | -0.595958 | 1.703759  |
| 1  | -0.293253 | 0.356984  | 1.500313  |
| 1  | -1.518524 | -0.693268 | 1.291815  |
| 1  | -0.685891 | -0.682662 | 2.711679  |
| 7  | -1.477591 | 2.005586  | 0.000007  |
| 1  | -1.695535 | 2.580370  | -0.811140 |
| 1  | -2.143325 | 1.231638  | 0.000004  |
| 1  | -1.695542 | 2.580368  | 0.811155  |
| 7  | -3.537594 | -0.645861 | -0.000010 |
| 1  | -4.068089 | -0.330910 | -0.810296 |
| 1  | -4.068088 | -0.330941 | 0.810288  |
| 1  | -3.613917 | -1.661235 | -0.000029 |
| 7  | -0.590564 | -0.595949 | -1.703755 |
| 1  | -0.293238 | 0.356990  | -1.500304 |
| 1  | -0.685878 | -0.682648 | -2.711675 |
| 1  | -1.518518 | -0.693255 | -1.291816 |
| 7  | 1.778485  | 2.155561  | 0.000000  |
| 1  | 2.051190  | 2.703802  | 0.811944  |
| 1  | 2.051178  | 2.703809  | -0.811944 |

1      0.757878      2.109641      0.000008

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Cartesian coordinates of :      BL7\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.955330 | -0.597772 | 0.557030  |
| 1  | -1.010249 | -0.160003 | 0.104578  |
| 1  | -2.757420 | 0.061337  | 0.457598  |
| 1  | -2.191831 | -1.508214 | 0.106204  |
| 1  | -1.797442 | -0.763688 | 1.549426  |
| 7  | -2.613202 | -3.195593 | -0.700247 |
| 1  | -1.888904 | -3.891339 | -0.540984 |
| 1  | -2.724218 | -3.122042 | -1.708323 |
| 1  | -3.478119 | -3.594818 | -0.344386 |
| 7  | 0.302120  | 0.411932  | -0.461690 |
| 1  | 0.329636  | 1.439510  | -0.452696 |
| 1  | 1.102555  | 0.071929  | 0.096784  |
| 1  | 0.472042  | 0.124637  | -1.422928 |
| 7  | 5.322595  | -0.840425 | -0.409259 |
| 1  | 5.971048  | -1.396847 | 0.140485  |
| 1  | 5.252110  | -1.286889 | -1.318908 |
| 1  | 5.766455  | 0.060963  | -0.559183 |
| 7  | 2.632785  | -0.615153 | 1.232276  |
| 1  | 3.479362  | -0.676874 | 0.656331  |
| 1  | 2.507714  | -1.528270 | 1.660861  |
| 1  | 2.845967  | 0.025836  | 1.991966  |
| 7  | 0.531248  | 3.541630  | -0.499231 |
| 1  | -0.109943 | 4.046573  | -1.104267 |
| 1  | 0.481160  | 3.984206  | 0.413954  |
| 1  | 1.465936  | 3.720345  | -0.856152 |
| 7  | -4.237011 | 1.271805  | 0.318662  |
| 1  | -4.485981 | 1.462676  | -0.648540 |
| 1  | -4.032635 | 2.171562  | 0.745923  |
| 1  | -5.079689 | 0.924448  | 0.769471  |

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Cartesian coordinates of :      BTC7\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.336808  | -0.123940 | 1.074229  |
| 1  | 0.863390  | 0.058037  | 1.927062  |
| 1  | -0.673730 | -0.363824 | 1.312285  |
| 1  | 0.388874  | 0.728843  | 0.479596  |
| 1  | 0.788555  | -0.923074 | 0.552713  |
| 7  | -1.459969 | -1.278484 | -1.512809 |
| 1  | -2.223532 | -1.947676 | -1.451227 |
| 1  | -1.322090 | -1.110570 | -2.506699 |
| 1  | -1.800817 | -0.401906 | -1.114921 |
| 7  | -2.261573 | 1.733048  | -0.482207 |
| 1  | -2.734877 | 2.369619  | 0.155187  |
| 1  | -2.669131 | 1.909467  | -1.397553 |
| 1  | -1.288350 | 2.035889  | -0.524998 |
| 7  | 1.062222  | 2.258785  | -0.480697 |
| 1  | 1.975634  | 1.846641  | -0.261475 |
| 1  | 1.029588  | 2.377568  | -1.490379 |
| 1  | 1.051866  | 3.194173  | -0.081023 |
| 7  | 1.273106  | -2.323308 | -0.465133 |
| 1  | 1.993578  | -2.326250 | -1.182341 |
| 1  | 1.310872  | -3.232665 | -0.011955 |
| 1  | 0.369319  | -2.245481 | -0.944365 |
| 7  | 3.420647  | 0.348031  | 0.353428  |
| 1  | 3.910762  | 0.480211  | 1.234694  |
| 1  | 3.164904  | -0.636132 | 0.300715  |
| 1  | 4.115582  | 0.502167  | -0.373512 |
| 7  | -2.374269 | -0.655313 | 1.596159  |

|   |           |           |          |
|---|-----------|-----------|----------|
| 1 | -2.757060 | -0.428066 | 2.510136 |
| 1 | -2.776217 | -0.006246 | 0.917750 |
| 1 | -2.695926 | -1.592457 | 1.369520 |

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Cartesian coordinates of : TC7\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.009092  | -0.014184 | -0.560704 |
| 1  | 1.003750  | -0.061924 | -0.213870 |
| 1  | 0.028614  | -0.046716 | -1.579336 |
| 1  | -0.546625 | -0.842630 | -0.216899 |
| 1  | -0.447427 | 0.891506  | -0.268483 |
| 7  | -1.778596 | -2.105233 | 0.273158  |
| 1  | -2.066567 | -2.874923 | -0.326782 |
| 1  | -1.767894 | -2.468422 | 1.223412  |
| 1  | -2.526971 | -1.399357 | 0.229528  |
| 7  | 2.721490  | -0.490750 | 0.271889  |
| 1  | 2.487257  | -1.489741 | 0.191392  |
| 1  | 3.535407  | -0.331292 | -0.317427 |
| 1  | 3.023397  | -0.332151 | 1.230364  |
| 7  | -0.941789 | 2.604893  | 0.137635  |
| 1  | -1.439814 | 3.205919  | -0.514975 |
| 1  | -1.299248 | 2.825083  | 1.064351  |
| 1  | 0.044878  | 2.898723  | 0.120364  |
| 7  | 1.408941  | -3.222858 | -0.111230 |
| 1  | 1.579300  | -3.675869 | -1.004933 |
| 1  | 0.403119  | -3.096364 | -0.022100 |
| 1  | 1.691162  | -3.887150 | 0.604678  |
| 7  | -3.512873 | 0.387266  | -0.012511 |
| 1  | -4.098316 | 0.422498  | -0.842536 |
| 1  | -4.132798 | 0.519754  | 0.782136  |
| 1  | -2.892024 | 1.192772  | -0.045020 |
| 7  | 2.094003  | 2.842102  | -0.007616 |
| 1  | 2.464950  | 3.268364  | -0.852324 |
| 1  | 2.475025  | 3.371274  | 0.772232  |
| 1  | 2.478962  | 1.902000  | 0.051880  |

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Cartesian coordinates of : BL7\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.000950 | -0.011608 | -1.037736 |
| 1  | -0.922831 | -0.052940 | -0.412237 |
| 1  | -0.041330 | 0.806655  | -1.643044 |
| 1  | 0.921101  | 0.037716  | -0.413095 |
| 1  | 0.039251  | -0.837579 | -1.632502 |
| 7  | 2.244727  | 0.108829  | 0.462745  |
| 1  | 2.049762  | 0.368560  | 1.427135  |
| 1  | 2.734105  | -0.795158 | 0.495354  |
| 1  | 2.906755  | 0.806842  | 0.099051  |
| 7  | -2.246314 | -0.113060 | 0.464612  |
| 1  | -2.729013 | 0.794535  | 0.496462  |
| 1  | -2.913628 | -0.806612 | 0.102036  |
| 1  | -2.052804 | -0.373111 | 1.429211  |
| 7  | -3.754124 | 2.623303  | 0.630680  |
| 1  | -4.197022 | 2.905372  | -0.239335 |
| 1  | -4.501207 | 2.504107  | 1.309517  |
| 1  | -3.202052 | 3.415960  | 0.945965  |
| 7  | -4.300112 | -2.234773 | -0.569892 |
| 1  | -4.641315 | -2.072019 | -1.513143 |
| 1  | -5.109318 | -2.181610 | 0.042893  |
| 1  | -3.978872 | -3.198347 | -0.539556 |
| 7  | 4.284374  | 2.243189  | -0.574059 |
| 1  | 5.052775  | 2.260519  | 0.091101  |
| 1  | 3.934164  | 3.195173  | -0.634211 |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 4.691275 | 2.025724  | -1.479481 |
| 7 | 3.772210 | -2.616420 | 0.630821  |
| 1 | 4.206969 | -2.903559 | -0.241633 |
| 1 | 4.526163 | -2.486975 | 1.300118  |
| 1 | 3.228407 | -3.409484 | 0.959202  |

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Cartesian coordinates of : BL7\_7

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.346177 | 0.137701  | -0.413647 |
| 1  | -2.781415 | -0.805929 | -0.540396 |
| 1  | -2.018454 | 0.467551  | -1.320172 |
| 1  | -3.056732 | 0.813996  | -0.048503 |
| 1  | -1.481831 | 0.074860  | 0.268668  |
| 7  | -4.321358 | 2.056715  | 0.592750  |
| 1  | -5.133257 | 2.143412  | -0.013689 |
| 1  | -4.675559 | 1.802859  | 1.511718  |
| 1  | -3.931657 | 2.991714  | 0.684453  |
| 7  | -3.535989 | -2.513008 | -0.797624 |
| 1  | -4.291561 | -2.514837 | -1.478475 |
| 1  | -2.848828 | -3.185085 | -1.130240 |
| 1  | -3.922219 | -2.898592 | 0.060571  |
| 7  | -0.159120 | -0.010258 | 1.199472  |
| 1  | 0.682759  | -0.050596 | 0.583268  |
| 1  | -0.128486 | -0.832659 | 1.797873  |
| 1  | -0.037951 | 0.791677  | 1.813995  |
| 7  | 3.816457  | 2.652784  | -0.692289 |
| 1  | 4.590261  | 2.483751  | -1.328534 |
| 1  | 3.332044  | 3.477676  | -1.033366 |
| 1  | 4.223398  | 2.900750  | 0.204758  |
| 7  | 2.213456  | -0.118506 | -0.545928 |
| 1  | 2.874337  | -0.790099 | -0.143612 |
| 1  | 2.073829  | -0.400205 | -1.512626 |
| 1  | 2.686731  | 0.789350  | -0.575096 |
| 7  | 4.333669  | -2.200836 | 0.643680  |
| 1  | 5.160715  | -2.139741 | 0.056870  |
| 1  | 4.627840  | -1.976088 | 1.589540  |
| 1  | 4.049469  | -3.175915 | 0.648100  |

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Cartesian coordinates of : BL7\_8

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -4.130814 | 0.066518  | -1.086160 |
| 1  | -2.525351 | -0.001640 | 0.079903  |
| 1  | -4.211135 | -0.708731 | -1.738770 |
| 1  | -4.963727 | 0.032900  | -0.487477 |
| 1  | -4.207245 | 0.913868  | -1.642548 |
| 7  | -6.746069 | -0.033770 | 0.662015  |
| 1  | -6.861948 | -0.901264 | 1.177789  |
| 1  | -6.825189 | 0.721268  | 1.337019  |
| 1  | -7.545696 | 0.045346  | 0.040112  |
| 7  | -1.688961 | -0.035214 | 0.689933  |
| 1  | -1.777889 | -0.870000 | 1.264711  |
| 1  | -0.282973 | -0.015763 | -0.256279 |
| 1  | -1.758659 | 0.754671  | 1.327378  |
| 7  | 4.579190  | -2.507901 | 0.010850  |
| 1  | 4.944991  | -2.579191 | -0.934696 |
| 1  | 5.385585  | -2.451489 | 0.627310  |
| 1  | 4.125193  | -3.394450 | 0.213032  |
| 7  | 0.596011  | -0.002488 | -0.885404 |
| 1  | 0.562971  | 0.827081  | -1.475830 |
| 1  | 0.573296  | -0.817386 | -1.496392 |
| 1  | 1.575602  | -0.004253 | -0.258419 |
| 7  | 2.828207  | -0.006534 | 0.537231  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 3.407858 | -0.835129 | 0.338385  |
| 1 | 3.400533 | 0.830893  | 0.354882  |
| 1 | 2.633729 | -0.017306 | 1.536403  |
| 7 | 4.557622 | 2.519670  | 0.060379  |
| 1 | 4.091559 | 3.400147  | 0.261611  |
| 1 | 4.937219 | 2.601360  | -0.878868 |
| 1 | 5.354970 | 2.467090  | 0.688834  |

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Cartesian coordinates of : TC7\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.339361  | -1.426717 | 1.180098  |
| 1  | 3.351271  | -1.347885 | 1.094119  |
| 1  | 1.868894  | -0.403177 | 1.259331  |
| 1  | 1.934614  | -1.925284 | 0.307026  |
| 1  | 2.133770  | -1.974075 | 2.014206  |
| 7  | 1.171422  | -2.498148 | -1.067414 |
| 1  | 1.769280  | -2.655418 | -1.874509 |
| 1  | 0.622344  | -3.344645 | -0.943613 |
| 1  | 0.526408  | -1.727026 | -1.294088 |
| 7  | 1.502704  | 2.711708  | -1.365379 |
| 1  | 1.866905  | 2.366213  | -2.250036 |
| 1  | 0.707809  | 3.304315  | -1.592973 |
| 1  | 2.216815  | 3.334493  | -0.994729 |
| 7  | -3.679953 | -0.608392 | -0.424638 |
| 1  | -4.464257 | -0.926091 | 0.139650  |
| 1  | -4.060387 | 0.070156  | -1.079349 |
| 1  | -3.383704 | -1.410608 | -0.974445 |
| 7  | -0.532870 | 0.022720  | -1.352960 |
| 1  | -1.233130 | 0.072201  | -0.614303 |
| 1  | -1.028577 | 0.128303  | -2.234194 |
| 1  | 0.070822  | 0.837948  | -1.255053 |
| 7  | -1.854919 | 0.733884  | 1.797405  |
| 1  | -2.193275 | 1.687179  | 1.902064  |
| 1  | -2.485019 | 0.269678  | 1.137560  |
| 1  | -1.991001 | 0.286200  | 2.700138  |
| 7  | 1.169672  | 0.980709  | 1.315068  |
| 1  | 1.310235  | 1.515346  | 0.451473  |
| 1  | 0.151426  | 0.868407  | 1.445394  |
| 1  | 1.500836  | 1.563415  | 2.081080  |

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Cartesian coordinates of : L7

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.000001  | -0.733036 | 0.180795  |
| 1  | -0.913500 | -0.116364 | 0.132846  |
| 1  | 0.913506  | -0.116364 | 0.132924  |
| 1  | -0.000036 | -1.268498 | 1.047832  |
| 1  | 0.000035  | -1.394954 | -0.594073 |
| 7  | -7.310885 | 0.648445  | -0.079011 |
| 1  | -7.388173 | 1.300489  | -0.854233 |
| 1  | -7.464411 | 1.184428  | 0.770271  |
| 1  | -8.091999 | 0.003727  | -0.161679 |
| 7  | -4.669846 | -1.049427 | -0.069568 |
| 1  | -4.715585 | -1.622733 | -0.907966 |
| 1  | -4.763686 | -1.688859 | 0.715241  |
| 1  | -5.512574 | -0.462733 | -0.070637 |
| 7  | -2.279812 | 0.752046  | 0.060968  |
| 1  | -3.107784 | 0.126819  | 0.017349  |
| 1  | -2.409278 | 1.358031  | 0.868327  |
| 1  | -2.323297 | 1.357115  | -0.756227 |
| 7  | 2.279825  | 0.752044  | 0.061154  |
| 1  | 2.323294  | 1.357250  | -0.755940 |
| 1  | 3.107790  | 0.126816  | 0.017406  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 2.409321 | 1.357894  | 0.868611  |
| 7 | 7.310879 | 0.648443  | -0.078949 |
| 1 | 7.464346 | 1.184393  | 0.770365  |
| 1 | 8.092003 | 0.003735  | -0.161592 |
| 1 | 7.388211 | 1.300519  | -0.854139 |
| 7 | 4.669838 | -1.049428 | -0.069762 |
| 1 | 4.763694 | -1.689003 | 0.714929  |
| 1 | 5.512570 | -0.462740 | -0.070746 |
| 1 | 4.715550 | -1.622582 | -0.908264 |

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Cartesian coordinates of the protonated ammonia octamer

Cartesian coordinates of : DC8\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.601906  | -0.002597 | -0.010229 |
| 1  | 1.309907  | -0.008256 | -1.026718 |
| 1  | 2.171432  | -0.845888 | 0.196389  |
| 1  | 2.166097  | 0.846127  | 0.188560  |
| 1  | 0.725955  | -0.002355 | 0.577160  |
| 7  | -2.744153 | 2.571388  | 0.706842  |
| 1  | -3.732726 | 2.362978  | 0.823556  |
| 1  | -2.676379 | 3.220847  | -0.072825 |
| 1  | -2.466419 | 3.095142  | 1.533277  |
| 7  | -2.262895 | 0.000079  | -1.385911 |
| 1  | -3.042290 | 0.002185  | -2.037852 |
| 1  | -2.370574 | -0.816389 | -0.785453 |
| 1  | -2.364024 | 0.819285  | -0.788051 |
| 7  | 0.542890  | -0.017712 | -2.649938 |
| 1  | -0.449411 | -0.011655 | -2.379274 |
| 1  | 0.708923  | 0.790856  | -3.242581 |
| 1  | 0.702571  | -0.837766 | -3.228398 |
| 7  | 3.287179  | 2.416527  | 0.524917  |
| 1  | 3.450247  | 2.584682  | 1.514155  |
| 1  | 2.875106  | 3.267371  | 0.151137  |
| 1  | 4.202944  | 2.326723  | 0.092448  |
| 7  | -2.758948 | -2.563747 | 0.711885  |
| 1  | -3.746861 | -2.350400 | 0.825249  |
| 1  | -2.692044 | -3.215878 | -0.065629 |
| 1  | -2.486045 | -3.086247 | 1.540720  |
| 7  | 3.305318  | -2.404463 | 0.543328  |
| 1  | 4.045065  | -2.490397 | -0.148879 |
| 1  | 2.783877  | -3.276675 | 0.517307  |
| 1  | 3.761661  | -2.368031 | 1.451050  |
| 7  | -0.865413 | -0.000501 | 1.476998  |
| 1  | -0.779030 | -0.000321 | 2.489921  |
| 1  | -1.421409 | -0.821053 | 1.225108  |
| 1  | -1.417764 | 0.822298  | 1.224379  |

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Cartesian coordinates of : BC8\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X        | Y         | Z         |
|----|----------|-----------|-----------|
| 7  | 1.966420 | -0.001708 | -0.114769 |
| 1  | 1.321283 | 0.681296  | 0.355139  |
| 1  | 1.405797 | -0.840267 | -0.440092 |
| 1  | 2.422840 | 0.451792  | -0.930928 |
| 1  | 2.695760 | -0.311192 | 0.558039  |
| 7  | 3.293525 | 1.270619  | -2.471801 |
| 1  | 2.639374 | 1.786265  | -3.054710 |
| 1  | 4.027224 | 1.925182  | -2.213207 |
| 1  | 3.727071 | 0.573965  | -3.072222 |
| 7  | 0.197141 | 1.899241  | 1.195797  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.430933  | 2.851607  | 0.925583  |
| 1 | -0.799461 | 1.771778  | 0.982925  |
| 1 | 0.283871  | 1.867766  | 2.208787  |
| 7 | 4.064642  | -0.915665 | 1.807963  |
| 1 | 3.670536  | -1.470935 | 2.562987  |
| 1 | 4.568745  | -0.149309 | 2.246389  |
| 1 | 4.763764  | -1.499551 | 1.356215  |
| 7 | 0.346566  | -2.201353 | -0.906541 |
| 1 | -0.528490 | -2.024444 | -0.393671 |
| 1 | 0.117470  | -2.250618 | -1.895570 |
| 1 | 0.674913  | -3.126102 | -0.641475 |
| 7 | -2.914048 | 1.724619  | 0.715979  |
| 1 | -3.412959 | 1.722519  | 1.602272  |
| 1 | -3.080077 | 2.638279  | 0.301620  |
| 1 | -3.378210 | 1.038328  | 0.118876  |
| 7 | -2.094841 | -1.385495 | 0.761950  |
| 1 | -2.920037 | -1.150439 | 0.210328  |
| 1 | -1.830571 | -0.529811 | 1.243658  |
| 1 | -2.381431 | -2.056679 | 1.468739  |
| 7 | -4.745436 | -0.438679 | -0.982570 |
| 1 | -5.551780 | -0.543466 | -0.371782 |
| 1 | -4.675803 | -1.302167 | -1.515574 |
| 1 | -4.988546 | 0.285162  | -1.654365 |

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Cartesian coordinates of : BC8\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.942046  | -0.624347 | -0.089940 |
| 1  | 0.650663  | -0.195094 | 0.817131  |
| 1  | 1.326062  | -1.577266 | 0.064549  |
| 1  | 0.058985  | -0.672762 | -0.648407 |
| 1  | 1.655469  | -0.019849 | -0.576966 |
| 7  | -1.739192 | -0.514420 | -1.191414 |
| 1  | -2.201533 | -1.395088 | -1.400438 |
| 1  | -2.247855 | -0.087057 | -0.412574 |
| 1  | -1.879158 | 0.083503  | -2.001347 |
| 7  | -0.414927 | 0.585543  | 2.169578  |
| 1  | -0.463003 | 0.061037  | 3.038730  |
| 1  | -0.147096 | 1.533829  | 2.418433  |
| 1  | -1.363157 | 0.627706  | 1.786514  |
| 7  | 2.870758  | 1.027145  | -1.448356 |
| 1  | 3.728948  | 1.193158  | -0.907924 |
| 1  | 2.486486  | 1.942157  | -1.670908 |
| 1  | 3.159097  | 0.620426  | -2.334864 |
| 7  | 2.048016  | -3.364775 | 0.337196  |
| 1  | 2.823222  | -3.368093 | 0.994922  |
| 1  | 1.357336  | -4.015643 | 0.701676  |
| 1  | 2.399700  | -3.770451 | -0.526156 |
| 7  | 5.534957  | 1.640176  | 0.066580  |
| 1  | 6.249185  | 0.933146  | -0.083340 |
| 1  | 5.902077  | 2.507324  | -0.315869 |
| 1  | 5.462898  | 1.773271  | 1.071196  |
| 7  | -5.677855 | 0.406358  | -1.031564 |
| 1  | -5.532340 | 0.927256  | -1.891700 |
| 1  | -6.544093 | 0.752442  | -0.627618 |
| 1  | -5.849781 | -0.558567 | -1.299346 |
| 7  | -3.490026 | 0.825424  | 1.178943  |
| 1  | -4.202430 | 0.685561  | 0.451973  |
| 1  | -3.516381 | 1.815720  | 1.411516  |
| 1  | -3.829725 | 0.335611  | 2.003656  |

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Cartesian coordinates of : BTC8\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 1.811245  | -0.253663 | 0.060758  |
| 1 | 1.309190  | -0.136992 | 0.968931  |
| 1 | 2.638169  | -0.879799 | 0.135289  |
| 1 | 1.089488  | -0.601079 | -0.606168 |
| 1 | 2.064292  | 0.705433  | -0.283689 |
| 7 | 1.872590  | 2.415427  | -0.947487 |
| 1 | 2.353769  | 3.164457  | -0.457579 |
| 1 | 0.865914  | 2.557061  | -0.822866 |
| 1 | 2.083554  | 2.532359  | -1.934663 |
| 7 | -0.043151 | 0.289958  | 2.222607  |
| 1 | -0.162667 | -0.353725 | 3.000126  |
| 1 | 0.095681  | 1.211196  | 2.629434  |
| 1 | -0.927503 | 0.317150  | 1.710892  |
| 7 | -3.015204 | 0.121143  | 0.825315  |
| 1 | -2.897936 | -0.807297 | 0.412409  |
| 1 | -3.768496 | 0.565677  | 0.304474  |
| 1 | -3.379428 | -0.014063 | 1.765803  |
| 7 | -1.237648 | 2.609061  | -0.205144 |
| 1 | -1.810853 | 3.007655  | -0.945125 |
| 1 | -1.101973 | 3.356546  | 0.471499  |
| 1 | -1.802434 | 1.891738  | 0.255361  |
| 7 | 4.208557  | -1.984757 | 0.260800  |
| 1 | 4.101575  | -2.764999 | 0.903807  |
| 1 | 4.471294  | -2.384276 | -0.636559 |
| 1 | 5.012252  | -1.452744 | 0.585013  |
| 7 | -0.582925 | -0.425388 | -1.516520 |
| 1 | -0.806890 | 0.537207  | -1.263187 |
| 1 | -1.338050 | -1.016079 | -1.168883 |
| 1 | -0.591875 | -0.484304 | -2.530867 |
| 7 | -2.822804 | -2.728746 | -0.705689 |
| 1 | -3.449255 | -3.166778 | -0.034189 |
| 1 | -2.052394 | -3.380222 | -0.834588 |
| 1 | -3.330034 | -2.705364 | -1.587145 |

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Cartesian coordinates of : BDC8\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.914321 | -0.051989 | 0.006165  |
| 1  | -2.241548 | -0.644644 | 0.794414  |
| 1  | -0.966517 | -0.361732 | -0.335408 |
| 1  | -2.608318 | -0.077900 | -0.767447 |
| 1  | -1.765579 | 0.938431  | 0.331821  |
| 7  | -2.912014 | -1.693336 | 2.291179  |
| 1  | -2.199564 | -1.849384 | 2.999445  |
| 1  | -3.685205 | -1.226919 | 2.758668  |
| 1  | -3.252702 | -2.611109 | 2.016973  |
| 7  | -1.060973 | 2.568191  | 0.772870  |
| 1  | -1.405556 | 3.345913  | 0.216261  |
| 1  | -1.188256 | 2.834052  | 1.745761  |
| 1  | -0.050115 | 2.499848  | 0.606852  |
| 7  | 2.075754  | 2.494181  | 0.340132  |
| 1  | 2.278766  | 2.956198  | 1.223580  |
| 1  | 2.234925  | 3.192744  | -0.382058 |
| 1  | 2.799812  | 1.776074  | 0.216516  |
| 7  | -3.918474 | -0.101516 | -2.201857 |
| 1  | -4.025394 | -1.020709 | -2.622966 |
| 1  | -4.842420 | 0.178898  | -1.883169 |
| 1  | -3.669771 | 0.533367  | -2.956075 |
| 7  | 0.790788  | -0.367536 | -0.841162 |
| 1  | 1.401689  | -1.134509 | -0.553623 |
| 1  | 0.907141  | -0.274795 | -1.847426 |
| 1  | 1.173786  | 0.485712  | -0.428847 |
| 7  | 2.783393  | -2.909822 | -0.218340 |
| 1  | 3.159772  | -3.133126 | 0.699655  |
| 1  | 2.011651  | -3.554111 | -0.372007 |
| 1  | 3.500910  | -3.164598 | -0.892786 |
| 7  | 4.077987  | 0.157048  | -0.141772 |
| 1  | 3.622580  | -0.754287 | -0.164469 |

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1      4.797147      0.122545      0.575186
1      4.557778      0.277502     -1.029358
-----

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Cartesian coordinates of : BL8\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.000658 | -0.408221 | -0.139501 |
| 1  | -0.858591 | -0.461227 | 0.464846  |
| 1  | -0.006658 | -1.193802 | -0.817255 |
| 1  | 0.008211  | 0.502848  | -0.662641 |
| 1  | 0.854346  | -0.476435 | 0.467455  |
| 7  | 0.024458  | 2.091208  | -1.619383 |
| 1  | -0.780080 | 2.169657  | -2.236439 |
| 1  | 0.019189  | 2.927932  | -1.023695 |
| 1  | 0.845126  | 2.164955  | -2.215432 |
| 7  | -2.334133 | -0.549222 | 1.583755  |
| 1  | -2.498910 | 0.344776  | 2.039689  |
| 1  | -3.210212 | -0.803085 | 1.111677  |
| 1  | -2.200958 | -1.225998 | 2.331131  |
| 7  | 2.324499  | -0.591759 | 1.591164  |
| 1  | 3.202207  | -0.835607 | 1.116795  |
| 1  | 2.187768  | -1.285337 | 2.322314  |
| 1  | 2.488484  | 0.291298  | 2.068207  |
| 7  | 0.012099  | 4.758971  | 0.027000  |
| 1  | 0.784435  | 4.873555  | 0.677030  |
| 1  | -0.839835 | 4.929835  | 0.553533  |
| 1  | 0.089577  | 5.511802  | -0.651373 |
| 7  | 5.104108  | -1.322839 | 0.338244  |
| 1  | 5.382204  | -0.789135 | -0.480275 |
| 1  | 5.794675  | -1.130627 | 1.058736  |
| 1  | 5.205358  | -2.304150 | 0.095143  |
| 7  | -0.019679 | -2.684378 | -2.098885 |
| 1  | -0.873085 | -2.711956 | -2.650367 |
| 1  | 0.751013  | -2.634819 | -2.759785 |
| 1  | 0.054367  | -3.585212 | -1.633778 |
| 7  | -5.110394 | -1.307340 | 0.338464  |
| 1  | -5.800931 | -1.107209 | 1.056831  |
| 1  | -5.390194 | -0.785000 | -0.486782 |
| 1  | -5.209607 | -2.292000 | 0.108423  |

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Cartesian coordinates of : BC8\_3

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.000384 | -0.594212 | 0.065185  |
| 1  | -0.000236 | 0.051253  | 0.880203  |
| 1  | -0.858748 | -1.202535 | 0.072943  |
| 1  | -0.000070 | 0.033164  | -0.765211 |
| 1  | 0.857597  | -1.203074 | 0.073121  |
| 7  | 0.001061  | 1.621755  | -1.858841 |
| 1  | -0.813776 | 1.707599  | -2.459952 |
| 1  | 0.001602  | 2.426920  | -1.230004 |
| 1  | 0.816214  | 1.706334  | -2.459704 |
| 7  | 0.000615  | 1.689853  | 1.916564  |
| 1  | -0.814504 | 1.807399  | 2.511733  |
| 1  | 0.815761  | 1.806177  | 2.511935  |
| 1  | 0.001284  | 2.457529  | 1.243431  |
| 7  | 2.283116  | -2.369113 | 0.096167  |
| 1  | 2.296911  | -2.914038 | 0.954920  |
| 1  | 3.207869  | -1.929527 | 0.014794  |
| 1  | 2.216231  | -3.042744 | -0.663021 |
| 7  | -2.284865 | -2.367845 | 0.095706  |
| 1  | -2.298867 | -2.913010 | 0.954302  |
| 1  | -3.209415 | -1.927802 | 0.014513  |
| 1  | -2.218339 | -3.041286 | -0.663683 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 5.202608  | -1.260592 | -0.142561 |
| 1 | 5.805101  | -2.077956 | -0.099164 |
| 1 | 5.417646  | -0.787656 | -1.015624 |
| 1 | 5.499180  | -0.641479 | 0.606352  |
| 7 | -5.203918 | -1.258027 | -0.142527 |
| 1 | -5.418845 | -0.784750 | -1.015432 |
| 1 | -5.500201 | -0.639029 | 0.606595  |
| 1 | -5.806713 | -2.075179 | -0.099328 |
| 7 | 0.001808  | 4.377098  | -0.024069 |
| 1 | 0.009096  | 4.822274  | -0.939089 |
| 1 | 0.811466  | 4.745199  | 0.469738  |
| 1 | -0.816535 | 4.743799  | 0.456261  |

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Cartesian coordinates of : BC8\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -5.631949 | 0.176007  | 0.299261  |
| 1  | -5.832094 | -0.401605 | -0.512203 |
| 1  | -3.705234 | 1.027048  | 0.390871  |
| 1  | -6.308073 | 0.934768  | 0.288587  |
| 1  | -5.841524 | -0.387751 | 1.118243  |
| 7  | -1.986040 | -1.510956 | -0.796034 |
| 1  | -2.408427 | -2.218156 | -0.200163 |
| 1  | 0.021712  | -1.773543 | -1.413212 |
| 1  | -2.471032 | -1.570012 | -1.687816 |
| 7  | -2.759224 | 1.425399  | 0.429477  |
| 1  | -2.649297 | 1.996846  | -0.404684 |
| 1  | -2.757187 | 2.074964  | 1.212659  |
| 1  | -2.218539 | -0.602487 | -0.391830 |
| 7  | -0.194939 | -0.119946 | 1.561259  |
| 1  | -0.976527 | 0.410350  | 1.163028  |
| 1  | -0.203074 | 0.038282  | 2.565293  |
| 1  | -0.417931 | -1.101897 | 1.413770  |
| 7  | 0.995654  | -1.819625 | -1.737600 |
| 1  | 0.990856  | -1.621127 | -2.734568 |
| 1  | 1.302201  | -2.784005 | -1.640595 |
| 1  | 1.906706  | -0.614617 | -0.717399 |
| 7  | 2.885093  | 2.707982  | -1.215406 |
| 1  | 3.742757  | 3.099119  | -0.834400 |
| 1  | 2.161313  | 3.407199  | -1.071449 |
| 1  | 3.022627  | 2.636628  | -2.220247 |
| 7  | 4.618143  | -0.955267 | 1.443825  |
| 1  | 4.423868  | -1.819735 | 1.942533  |
| 1  | 5.382436  | -1.157649 | 0.804480  |
| 1  | 4.982887  | -0.302086 | 2.132322  |
| 7  | 2.212996  | 0.076566  | 0.017259  |
| 1  | 2.427789  | 0.997979  | -0.412853 |
| 1  | 3.050244  | -0.279709 | 0.520715  |
| 1  | 1.395408  | 0.150083  | 0.674626  |

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Cartesian coordinates of : BDC8\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.712807 | -0.529436 | 0.356133  |
| 1  | -0.770160 | -1.455440 | -0.113173 |
| 1  | 0.187520  | -0.466089 | 0.884813  |
| 1  | -0.733963 | 0.210782  | -0.368625 |
| 1  | -1.535957 | -0.406939 | 1.013920  |
| 7  | -3.003095 | -0.023027 | 1.938193  |
| 1  | -2.892524 | 0.407839  | 2.851713  |
| 1  | -3.710277 | -0.745359 | 2.040656  |
| 1  | -3.364917 | 0.688657  | 1.292853  |
| 7  | 2.104965  | -0.395826 | -1.389073 |
| 1  | 2.651099  | -0.583762 | -2.225834 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.879179  | -1.299426 | -0.981228 |
| 1 | 2.721280  | 0.076690  | -0.727713 |
| 7 | 4.280821  | 1.176978  | 0.565306  |
| 1 | 4.540162  | 1.558302  | 1.472378  |
| 1 | 5.065763  | 0.600633  | 0.270961  |
| 1 | 4.252533  | 1.970135  | -0.071046 |
| 7 | -3.346509 | 1.922104  | -0.408855 |
| 1 | -4.112556 | 1.724867  | -1.046376 |
| 1 | -3.426488 | 2.902359  | -0.153932 |
| 1 | -2.477927 | 1.811786  | -0.929937 |
| 7 | 1.783099  | -0.388741 | 1.897262  |
| 1 | 2.167320  | -1.297075 | 2.145917  |
| 1 | 1.569910  | 0.075820  | 2.776771  |
| 1 | 2.539119  | 0.141843  | 1.457088  |
| 7 | -0.371515 | 1.422182  | -1.896387 |
| 1 | -0.793376 | 1.320807  | -2.816044 |
| 1 | -0.152411 | 2.409193  | -1.787429 |
| 1 | 0.520889  | 0.915160  | -1.914192 |
| 7 | -0.910065 | -3.182638 | -0.998250 |
| 1 | -0.396851 | -3.937237 | -0.549808 |
| 1 | -0.614779 | -3.168361 | -1.971149 |
| 1 | -1.886852 | -3.466365 | -1.000878 |

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Cartesian coordinates of : BTC8\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.369125  | -3.302902 | -0.029145 |
| 1  | 1.511885  | -1.592579 | 0.189669  |
| 1  | 3.209203  | -3.356931 | 0.541407  |
| 1  | 1.780872  | -4.083125 | 0.251532  |
| 1  | 2.658563  | -3.488282 | -0.986004 |
| 7  | 1.099872  | -0.649527 | 0.346147  |
| 1  | 0.280406  | -0.698202 | 1.000204  |
| 1  | 1.842237  | 0.018385  | 0.698748  |
| 1  | 0.692381  | -0.273370 | -0.522649 |
| 7  | 1.745618  | 2.293870  | -1.605246 |
| 1  | 1.508126  | 3.281321  | -1.634483 |
| 1  | 0.876087  | 1.768087  | -1.677570 |
| 1  | 2.286272  | 2.102568  | -2.444080 |
| 7  | -1.083574 | 0.480937  | -1.352589 |
| 1  | -1.611248 | -0.379945 | -1.193377 |
| 1  | -1.456923 | 1.160738  | -0.685311 |
| 1  | -1.338419 | 0.803257  | -2.283023 |
| 7  | 3.053257  | 1.287066  | 1.008890  |
| 1  | 4.037240  | 1.037821  | 0.966545  |
| 1  | 2.933666  | 1.869823  | 1.832314  |
| 1  | 2.830203  | 1.849485  | 0.181256  |
| 7  | -1.471636 | -0.561318 | 1.596331  |
| 1  | -1.758385 | 0.411187  | 1.478655  |
| 1  | -2.042325 | -1.116359 | 0.955957  |
| 1  | -1.703539 | -0.840962 | 2.544824  |
| 7  | -2.392254 | 2.551157  | 0.891421  |
| 1  | -3.359565 | 2.398579  | 1.166885  |
| 1  | -1.924970 | 2.956387  | 1.698950  |
| 1  | -2.416652 | 3.285023  | 0.187292  |
| 7  | -3.124066 | -2.111721 | -0.779860 |
| 1  | -2.839451 | -2.545421 | -1.654835 |
| 1  | -3.388421 | -2.877956 | -0.164949 |
| 1  | -3.981638 | -1.602464 | -0.979593 |

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Cartesian coordinates of : BC8\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X        | Y         | Z        |
|----|----------|-----------|----------|
| 7  | 0.626950 | -0.089165 | 0.312833 |

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|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.516854  | -0.127140 | 1.344867  |
| 1 | 1.138618  | -0.950758 | -0.014608 |
| 1 | -0.339009 | -0.034504 | -0.155520 |
| 1 | 1.173296  | 0.747121  | 0.057806  |
| 7 | -1.874548 | 0.047820  | -0.932668 |
| 1 | -2.416967 | -0.806128 | -0.759399 |
| 1 | -2.452864 | 0.842670  | -0.640435 |
| 1 | -1.778699 | 0.120845  | -1.942918 |
| 7 | 0.296713  | -0.264578 | 3.283498  |
| 1 | 0.510876  | -1.204291 | 3.607133  |
| 1 | 0.887783  | 0.366180  | 3.818348  |
| 1 | -0.661062 | -0.073237 | 3.565433  |
| 7 | 4.243291  | 0.016176  | -0.806819 |
| 1 | 4.996718  | 0.016212  | -0.125539 |
| 1 | 4.669924  | 0.166756  | -1.716396 |
| 1 | 3.650834  | 0.818734  | -0.609070 |
| 7 | -3.570980 | -2.599631 | -0.570207 |
| 1 | -4.205176 | -2.654198 | -1.362336 |
| 1 | -3.023053 | -3.455058 | -0.577129 |
| 1 | -4.147375 | -2.629071 | 0.265870  |
| 7 | 2.210949  | -2.293530 | -0.606482 |
| 1 | 3.059528  | -1.737936 | -0.756192 |
| 1 | 2.438810  | -3.047971 | 0.034594  |
| 1 | 1.960421  | -2.727112 | -1.490526 |
| 7 | 1.933646  | 2.606686  | -0.497633 |
| 1 | 2.655329  | 3.086322  | 0.035288  |
| 1 | 2.168477  | 2.731431  | -1.479630 |
| 1 | 1.077691  | 3.136193  | -0.346760 |
| 7 | -3.810183 | 2.467269  | -0.217324 |
| 1 | -3.665135 | 3.041380  | 0.608037  |
| 1 | -4.722597 | 2.032419  | -0.111407 |
| 1 | -3.884089 | 3.103820  | -1.005910 |

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Cartesian coordinates of : Ca8

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.891539 | 2.193620  | -0.383624 |
| 1  | 0.197497  | 2.711607  | -0.155587 |
| 1  | -1.965697 | 2.615742  | -1.306959 |
| 1  | -2.355692 | 1.282348  | -0.446845 |
| 1  | -2.460179 | 2.774085  | 0.229035  |
| 7  | 0.009541  | -0.315405 | -1.465100 |
| 1  | -0.024553 | -0.270567 | -2.481481 |
| 1  | 0.303878  | 0.608165  | -1.149727 |
| 1  | -0.959127 | -0.406867 | -1.151029 |
| 7  | 2.181451  | 0.427121  | 1.064398  |
| 1  | 2.536309  | -0.318204 | 0.399734  |
| 1  | 2.839157  | 0.560218  | 1.829817  |
| 1  | 1.216638  | 0.160973  | 1.434752  |
| 7  | 1.217068  | 2.827225  | -0.168937 |
| 1  | 2.022431  | 1.334942  | 0.556941  |
| 1  | 1.481014  | 3.095258  | -1.113986 |
| 1  | 1.433779  | 3.628778  | 0.419190  |
| 7  | -3.055542 | -0.782567 | -0.260859 |
| 1  | -2.542807 | -1.591650 | 0.096132  |
| 1  | -3.568178 | -1.092744 | -1.083081 |
| 1  | -3.762253 | -0.557335 | 0.435862  |
| 7  | -0.698828 | -2.831260 | 0.399078  |
| 1  | -0.143847 | -3.208186 | 1.162852  |
| 1  | -0.069403 | -2.352974 | -0.244941 |
| 1  | -1.087154 | -3.633324 | -0.090734 |
| 7  | 2.866068  | -1.543069 | -0.842091 |
| 1  | 1.969221  | -1.488659 | -1.327718 |
| 1  | 3.013368  | -2.505531 | -0.550870 |
| 1  | 3.599906  | -1.325599 | -1.511004 |
| 7  | -0.495259 | 0.019584  | 1.755985  |
| 1  | -0.951212 | 0.750665  | 1.207883  |
| 1  | -0.788670 | 0.136610  | 2.722318  |

1      -0.865140      -0.874494      1.427501

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Cartesian coordinates of :      TC8\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.684486 | 0.605955  | -0.413951 |
| 1  | -0.221559 | 1.504695  | -0.206643 |
| 1  | -0.532177 | -0.057368 | 0.364755  |
| 1  | -1.727402 | 0.753570  | -0.559881 |
| 1  | -0.244123 | 0.155208  | -1.266256 |
| 7  | -3.484047 | 0.767776  | -0.653371 |
| 1  | -3.623507 | -0.062769 | -0.067287 |
| 1  | -4.002753 | 1.536606  | -0.238449 |
| 1  | -3.902616 | 0.588214  | -1.561743 |
| 7  | 0.521437  | 3.389603  | 0.100399  |
| 1  | 0.578277  | 3.772406  | 1.041569  |
| 1  | 1.367554  | 3.685726  | -0.381175 |
| 1  | -0.241224 | 3.888810  | -0.353520 |
| 7  | 0.625474  | -0.832286 | -2.476658 |
| 1  | 1.412377  | -1.244779 | -1.962024 |
| 1  | 0.078119  | -1.594507 | -2.867843 |
| 1  | 1.011497  | -0.323534 | -3.267655 |
| 7  | 2.994794  | -1.638285 | -0.622712 |
| 1  | 2.981843  | -0.933453 | 0.114241  |
| 1  | 3.807309  | -1.451780 | -1.205081 |
| 1  | 3.171049  | -2.536141 | -0.179454 |
| 7  | 0.405872  | -1.553185 | 1.326163  |
| 1  | 0.679347  | -2.193676 | 0.583281  |
| 1  | 1.215334  | -0.950554 | 1.491947  |
| 1  | 0.268734  | -2.110732 | 2.165389  |
| 7  | 2.467897  | 0.889882  | 1.495034  |
| 1  | 2.310894  | 1.029353  | 2.490459  |
| 1  | 3.437440  | 1.148029  | 1.327648  |
| 1  | 1.891264  | 1.573032  | 1.006783  |
| 7  | -2.993723 | -1.671692 | 1.157865  |
| 1  | -1.984922 | -1.713712 | 1.291058  |
| 1  | -3.286166 | -2.564826 | 0.771476  |
| 1  | -3.417111 | -1.602197 | 2.079026  |

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Cartesian coordinates of :      DC8\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.739907 | 1.896050  | -0.310591 |
| 1  | -2.432027 | 2.642069  | -0.340556 |
| 1  | -0.830607 | 2.270028  | 0.090740  |
| 1  | -2.093097 | 1.111067  | 0.299898  |
| 1  | -1.559065 | 1.527333  | -1.293193 |
| 7  | 0.721742  | 2.848165  | 0.744751  |
| 1  | 0.612184  | 3.420635  | 1.578510  |
| 1  | 1.191206  | 3.434698  | 0.058725  |
| 1  | 1.375859  | 2.091819  | 0.985216  |
| 7  | 2.682186  | 0.542522  | 1.464705  |
| 1  | 2.865642  | -0.150359 | 0.737344  |
| 1  | 2.457648  | 0.027038  | 2.311791  |
| 1  | 3.559191  | 1.022906  | 1.649420  |
| 7  | 0.276255  | -0.675149 | -0.326610 |
| 1  | 0.411632  | 0.025901  | 0.399318  |
| 1  | -0.357947 | -1.379907 | 0.046064  |
| 1  | 1.190762  | -1.109425 | -0.456422 |
| 7  | -1.032890 | 0.714987  | -2.742306 |
| 1  | -1.707819 | 0.183330  | -3.283831 |
| 1  | -0.449463 | 1.219269  | -3.403224 |
| 1  | -0.445091 | 0.062107  | -2.214041 |
| 7  | -2.662773 | -0.228663 | 1.392092  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -2.330416 | -0.121263 | 2.347444  |
| 1 | -3.678322 | -0.251024 | 1.446841  |
| 1 | -2.361853 | -1.155628 | 1.076022  |
| 7 | -1.809534 | -3.192520 | 0.552943  |
| 1 | -2.663483 | -3.604083 | 0.922532  |
| 1 | -1.762712 | -3.472178 | -0.423723 |
| 1 | -1.044111 | -3.664921 | 1.027620  |
| 7 | 3.415630  | -1.691300 | -0.839511 |
| 1 | 3.988560  | -1.054137 | -1.387501 |
| 1 | 4.052041  | -2.194754 | -0.226312 |
| 1 | 3.056330  | -2.379167 | -1.496995 |

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Cartesian coordinates of : BDC8\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.362745 | 0.425716  | -0.876556 |
| 1  | -0.420879 | -0.055493 | -0.981107 |
| 1  | -2.018653 | -0.103624 | -0.228615 |
| 1  | -1.129826 | 1.387129  | -0.492471 |
| 1  | -1.801573 | 0.520089  | -1.790165 |
| 7  | -6.142091 | -0.475017 | 0.062952  |
| 1  | -6.715737 | -0.952212 | 0.753208  |
| 1  | -6.430428 | 0.499382  | 0.072170  |
| 1  | -6.410745 | -0.848649 | -0.843097 |
| 7  | 1.317793  | -0.404155 | -1.065738 |
| 1  | 1.761558  | 0.375987  | -0.576845 |
| 1  | 1.673707  | -1.261982 | -0.637919 |
| 1  | 1.679524  | -0.388840 | -2.016496 |
| 7  | 4.318984  | -0.414326 | 0.494884  |
| 1  | 4.775792  | -0.522002 | 1.396187  |
| 1  | 3.736214  | -1.236919 | 0.346842  |
| 1  | 5.053442  | -0.434478 | -0.207141 |
| 7  | 2.555630  | -3.217334 | 0.046613  |
| 1  | 2.619387  | -3.452685 | 1.033997  |
| 1  | 3.379895  | -3.615111 | -0.397348 |
| 1  | 1.762205  | -3.739382 | -0.317331 |
| 7  | 2.766204  | 2.285715  | 0.350647  |
| 1  | 3.207102  | 2.852987  | -0.369597 |
| 1  | 2.871131  | 2.807394  | 1.217907  |
| 1  | 3.341132  | 1.440614  | 0.450726  |
| 7  | -0.328088 | 2.852351  | 0.122421  |
| 1  | 0.674428  | 2.633753  | 0.178008  |
| 1  | -0.425624 | 3.673221  | -0.469565 |
| 1  | -0.627745 | 3.132282  | 1.052752  |
| 7  | -3.167358 | -0.953668 | 0.819111  |
| 1  | -4.143504 | -0.775018 | 0.546699  |
| 1  | -3.041013 | -1.962795 | 0.807422  |
| 1  | -3.078098 | -0.668623 | 1.791434  |

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Cartesian coordinates of : BL8\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.281570  | -0.025762 | -0.755797 |
| 1  | 0.931305  | 0.605695  | -0.211166 |
| 1  | 0.160569  | 0.364022  | -1.688612 |
| 1  | 0.702436  | -0.990553 | -0.847696 |
| 1  | -0.688998 | -0.082440 | -0.275778 |
| 7  | 1.406034  | -2.649788 | -1.058862 |
| 1  | 2.173011  | -2.665007 | -1.726759 |
| 1  | 1.770794  | -3.047846 | -0.184340 |
| 1  | 0.713775  | -3.307033 | -1.410105 |
| 7  | 2.047278  | 1.702558  | 0.693689  |
| 1  | 2.745660  | 1.180211  | 1.216745  |
| 1  | 2.558835  | 2.353872  | 0.084799  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.546748  | 2.267874  | 1.374887  |
| 7 | -2.213051 | -0.179533 | 0.434078  |
| 1 | -2.933555 | -0.445071 | -0.247359 |
| 1 | -2.509931 | 0.703220  | 0.865399  |
| 1 | -2.239019 | -0.881981 | 1.169443  |
| 7 | 2.559227  | -4.022842 | 1.499889  |
| 1 | 2.064329  | -3.859412 | 2.371959  |
| 1 | 3.533454  | -3.788787 | 1.669111  |
| 1 | 2.528036  | -5.024706 | 1.331607  |
| 7 | -4.476245 | -1.023302 | -1.604167 |
| 1 | -4.260505 | -1.805147 | -2.215937 |
| 1 | -5.285881 | -1.299219 | -1.055474 |
| 1 | -4.777551 | -0.259543 | -2.202655 |
| 7 | -3.263238 | 2.457758  | 1.828284  |
| 1 | -3.105119 | 3.332815  | 1.337148  |
| 1 | -4.270373 | 2.339997  | 1.895577  |
| 1 | -2.923033 | 2.588418  | 2.776660  |
| 7 | 3.653613  | 3.713676  | -1.071236 |
| 1 | 4.270831  | 4.238215  | -0.457298 |
| 1 | 4.245628  | 3.275814  | -1.771438 |
| 1 | 3.082248  | 4.397226  | -1.559870 |

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Cartesian coordinates of : DC8\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.166707  | -2.964056 | -0.009845 |
| 1  | 0.764712  | -2.010606 | -0.494946 |
| 1  | 2.579834  | -3.566818 | -0.716180 |
| 1  | 2.840080  | -2.216898 | 0.200183  |
| 1  | 2.058275  | -3.530454 | 0.826970  |
| 7  | 0.046096  | -1.271304 | -0.752643 |
| 1  | 0.043567  | -1.146974 | -1.762891 |
| 1  | -0.919886 | -1.535353 | -0.438376 |
| 1  | 0.326404  | -0.343045 | -0.277099 |
| 7  | -5.005995 | 0.324051  | -0.143045 |
| 1  | -5.366955 | -0.042914 | -1.020533 |
| 1  | -5.254131 | 1.310651  | -0.131044 |
| 1  | -5.555383 | -0.110104 | 0.595036  |
| 7  | -2.244425 | 2.225967  | 0.284763  |
| 1  | -2.910633 | 1.465420  | 0.157963  |
| 1  | -2.517334 | 2.725881  | 1.126369  |
| 1  | -2.372894 | 2.869188  | -0.491247 |
| 7  | -2.645426 | -1.865034 | 0.155989  |
| 1  | -2.642860 | -2.116075 | 1.141373  |
| 1  | -3.085512 | -2.639014 | -0.335245 |
| 1  | -3.264673 | -1.057002 | 0.057133  |
| 7  | 0.653607  | 1.106506  | 0.523620  |
| 1  | 1.414315  | 1.664143  | 0.129898  |
| 1  | -0.225501 | 1.633269  | 0.463830  |
| 1  | 0.861128  | 0.976967  | 1.510526  |
| 7  | 3.241481  | 2.713078  | -0.571065 |
| 1  | 2.732717  | 3.576660  | -0.745112 |
| 1  | 3.962633  | 2.944451  | 0.107879  |
| 1  | 3.723277  | 2.491571  | -1.438840 |
| 7  | 3.867891  | -0.414926 | 0.493341  |
| 1  | 3.423676  | 0.432679  | 0.142636  |
| 1  | 4.775514  | -0.486635 | 0.041379  |
| 1  | 4.050081  | -0.268962 | 1.482532  |

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Cartesian coordinates of : BC8\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z        |
|----|-----------|-----------|----------|
| 7  | -1.185402 | -0.343730 | 1.404362 |
| 1  | -0.538250 | 0.486858  | 1.439256 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.786673 | -0.953077 | 0.614874  |
| 1 | -1.134519 | -0.849902 | 2.286011  |
| 1 | -2.191786 | -0.056813 | 1.226730  |
| 7 | 1.072654  | -4.605155 | -0.138236 |
| 1 | 1.668704  | -4.760003 | 0.669929  |
| 1 | 1.581620  | -4.954469 | -0.945523 |
| 1 | 0.264148  | -5.209826 | -0.022599 |
| 7 | -3.906471 | 0.385290  | 1.021708  |
| 1 | -4.517009 | -0.424553 | 1.101718  |
| 1 | -4.214357 | 1.040881  | 1.736157  |
| 1 | -4.117106 | 0.820938  | 0.114433  |
| 7 | 2.882768  | 0.220208  | -0.905695 |
| 1 | 2.777895  | 0.266550  | -1.916654 |
| 1 | 3.492124  | 1.005548  | -0.645921 |
| 1 | 3.417067  | -0.624858 | -0.716844 |
| 7 | 0.860146  | 1.623123  | 1.138039  |
| 1 | 1.473390  | 1.151376  | 0.465051  |
| 1 | 1.424798  | 1.840505  | 1.954902  |
| 1 | 0.592348  | 2.513670  | 0.727667  |
| 7 | 0.168154  | -1.647451 | -0.632832 |
| 1 | 0.491050  | -2.604849 | -0.447766 |
| 1 | -0.283509 | -1.657969 | -1.543543 |
| 1 | 0.990574  | -1.045386 | -0.711898 |
| 7 | 4.762646  | 2.611277  | -0.121951 |
| 1 | 5.160969  | 2.544155  | 0.810403  |
| 1 | 5.543504  | 2.582630  | -0.772049 |
| 1 | 4.355827  | 3.539010  | -0.199897 |
| 7 | -4.759491 | 1.715094  | -1.663725 |
| 1 | -4.299197 | 2.593404  | -1.885111 |
| 1 | -4.666939 | 1.122307  | -2.483721 |
| 1 | -5.749707 | 1.923276  | -1.567288 |

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Cartesian coordinates of : BL8\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.855428  | 0.171498  | -0.535048 |
| 1  | 1.572962  | 0.676103  | 0.061619  |
| 1  | 0.658811  | 0.740788  | -1.356262 |
| 1  | 1.236317  | -0.764584 | -0.856198 |
| 1  | -0.056851 | 0.036103  | 0.007978  |
| 7  | 1.868468  | -2.333198 | -1.448997 |
| 1  | 2.682264  | -2.220125 | -2.048732 |
| 1  | 2.149583  | -2.965927 | -0.688825 |
| 1  | 1.178299  | -2.834010 | -2.003660 |
| 7  | 2.786532  | 1.547190  | 1.042939  |
| 1  | 3.616153  | 0.981893  | 1.206310  |
| 1  | 3.105527  | 2.419901  | 0.601964  |
| 1  | 2.429416  | 1.797487  | 1.961790  |
| 7  | -1.576954 | -0.157049 | 0.830265  |
| 1  | -2.357772 | 0.124502  | 0.214287  |
| 1  | -1.653176 | 0.402719  | 1.676065  |
| 1  | -1.754585 | -1.118546 | 1.110419  |
| 7  | 2.767041  | -4.373648 | 0.730608  |
| 1  | 2.290579  | -5.256451 | 0.567456  |
| 1  | 2.607495  | -4.133251 | 1.704722  |
| 1  | 3.761429  | -4.561443 | 0.636569  |
| 7  | -3.878927 | 0.675356  | -0.978101 |
| 1  | -3.861951 | 1.653499  | -1.253984 |
| 1  | -3.952705 | 0.139098  | -1.838415 |
| 1  | -4.755534 | 0.530302  | -0.465311 |
| 7  | -6.625366 | 0.268999  | 0.517347  |
| 1  | -6.799473 | -0.688213 | 0.809361  |
| 1  | -6.728814 | 0.851262  | 1.343271  |
| 1  | -7.377710 | 0.523378  | -0.116342 |
| 7  | 3.819520  | 4.207295  | -0.201122 |
| 1  | 4.544183  | 4.565833  | 0.414907  |
| 1  | 4.240576  | 4.118678  | -1.121651 |
| 1  | 3.114787  | 4.935886  | -0.272577 |

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 Cartesian coordinates of : BC8\_7

-----  
 Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -4.454065 | -0.275753 | 0.883414  |
| 1  | -2.783726 | 0.198786  | -0.114874 |
| 1  | -4.560500 | 0.201310  | 1.774671  |
| 1  | -5.258201 | -0.003720 | 0.307216  |
| 1  | -4.558588 | -1.267907 | 1.078254  |
| 7  | -6.988539 | 0.522410  | -0.811249 |
| 1  | -7.055523 | 1.517064  | -1.006335 |
| 1  | -7.054118 | 0.042947  | -1.704386 |
| 1  | -7.818801 | 0.271129  | -0.282248 |
| 7  | -1.916387 | 0.438466  | -0.624631 |
| 1  | -1.934816 | 1.443110  | -0.782076 |
| 1  | -0.546659 | -0.104756 | 0.274612  |
| 1  | -1.985623 | 0.006616  | -1.542964 |
| 7  | 1.645657  | -2.611777 | -0.321719 |
| 1  | 2.605815  | -2.246334 | -0.369420 |
| 1  | 1.674243  | -3.482354 | 0.202515  |
| 1  | 1.361873  | -2.854600 | -1.267162 |
| 7  | 0.265023  | -0.471843 | 0.872565  |
| 1  | 0.724540  | -1.316457 | 0.411679  |
| 1  | -0.103836 | -0.750223 | 1.780059  |
| 1  | 0.994455  | 0.270877  | 1.017208  |
| 7  | 4.418655  | -1.248267 | -0.341213 |
| 1  | 4.339279  | -0.234151 | -0.398795 |
| 1  | 4.961244  | -1.463287 | 0.490557  |
| 1  | 4.974182  | -1.553577 | -1.135597 |
| 7  | 4.636144  | 2.025540  | -0.903533 |
| 1  | 5.616611  | 1.901342  | -0.661911 |
| 1  | 4.555251  | 1.814511  | -1.895338 |
| 1  | 4.452870  | 3.022463  | -0.814775 |
| 7  | 2.332631  | 1.515374  | 1.315223  |
| 1  | 1.956590  | 2.454099  | 1.423643  |
| 1  | 2.844783  | 1.315036  | 2.170854  |
| 1  | 3.024828  | 1.559025  | 0.562615  |

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Cartesian coordinates of : BC8\_8

-----  
 Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 3.977478  | -2.750891 | -0.308594 |
| 1  | 3.330017  | -3.502321 | -0.532425 |
| 1  | 4.614580  | -3.118744 | 0.393343  |
| 1  | 4.532500  | -2.591226 | -1.145453 |
| 1  | 3.056020  | -1.157495 | 0.272900  |
| 7  | 2.541567  | -0.307575 | 0.585028  |
| 1  | 2.127530  | -0.499061 | 1.495381  |
| 1  | 1.705790  | -0.039747 | -0.163137 |
| 1  | 3.206658  | 0.487517  | 0.687334  |
| 7  | -4.143212 | -1.983155 | 1.278731  |
| 1  | -4.453969 | -1.680056 | 2.198379  |
| 1  | -4.976171 | -2.284837 | 0.779455  |
| 1  | -3.582537 | -2.817388 | 1.432460  |
| 7  | -2.124450 | -1.011955 | -1.213268 |
| 1  | -2.606380 | -1.374543 | -0.391166 |
| 1  | -2.384117 | -1.599855 | -2.000125 |
| 1  | -2.524204 | -0.090052 | -1.376756 |
| 7  | 0.613410  | 0.318421  | -1.127750 |
| 1  | 0.956191  | 0.409746  | -2.081754 |
| 1  | 0.147630  | 1.208242  | -0.886416 |
| 1  | -0.155761 | -0.366698 | -1.150099 |
| 7  | 4.399466  | 1.990709  | 0.872015  |
| 1  | 5.188604  | 1.941832  | 0.232712  |

|   |           |          |           |
|---|-----------|----------|-----------|
| 1 | 4.791571  | 2.077535 | 1.806165  |
| 1 | 3.924298  | 2.868051 | 0.675909  |
| 7 | -1.215303 | 2.640172 | -0.403859 |
| 1 | -1.020072 | 3.221257 | 0.406540  |
| 1 | -1.395689 | 3.278201 | -1.174298 |
| 1 | -2.092623 | 2.146305 | -0.213008 |
| 7 | -3.971686 | 1.153541 | 0.254077  |
| 1 | -4.278162 | 1.750443 | 1.017724  |
| 1 | -4.706676 | 1.191325 | -0.447355 |
| 1 | -3.945926 | 0.196705 | 0.609032  |

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Cartesian coordinates of : TC8\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.590849 | -0.013928 | 0.458426  |
| 1  | -0.807767 | 0.975275  | 0.204170  |
| 1  | -0.413333 | -0.051414 | 1.460921  |
| 1  | -1.401124 | -0.641221 | 0.246076  |
| 1  | 0.302472  | -0.356367 | -0.063757 |
| 7  | -3.781996 | 1.403814  | 0.236187  |
| 1  | -4.220598 | 1.654520  | 1.118059  |
| 1  | -4.423671 | 1.694617  | -0.496596 |
| 1  | -2.942625 | 1.972891  | 0.142941  |
| 7  | 1.608346  | -1.091671 | -0.760260 |
| 1  | 2.510309  | -0.926476 | -0.307211 |
| 1  | 1.736439  | -0.960883 | -1.759949 |
| 1  | 1.319385  | -2.063030 | -0.605676 |
| 7  | -0.193590 | -3.494658 | -0.072857 |
| 1  | -0.250243 | -4.181842 | -0.819590 |
| 1  | -0.050868 | -4.016509 | 0.787186  |
| 1  | -1.105899 | -3.046647 | -0.008496 |
| 7  | -0.745179 | 2.833995  | -0.172685 |
| 1  | -1.055257 | 3.196882  | -1.071014 |
| 1  | -0.958048 | 3.551484  | 0.516254  |
| 1  | 0.279570  | 2.758437  | -0.220152 |
| 7  | -3.017956 | -1.562989 | -0.024922 |
| 1  | -3.493266 | -0.654061 | 0.046727  |
| 1  | -3.441267 | -2.176421 | 0.667215  |
| 1  | -3.251860 | -1.949843 | -0.936047 |
| 7  | 2.280583  | 2.181633  | -0.329741 |
| 1  | 2.511325  | 2.185593  | -1.320221 |
| 1  | 2.827308  | 2.927460  | 0.093281  |
| 1  | 2.636811  | 1.303134  | 0.044796  |
| 7  | 4.367936  | -0.294847 | 0.652010  |
| 1  | 4.721159  | -1.244173 | 0.748800  |
| 1  | 4.447338  | 0.127350  | 1.573835  |
| 1  | 5.032651  | 0.191808  | 0.055343  |

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Cartesian coordinates of : BC8\_9

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Atomic number (AN) and Cartesian coordinates

| AN | X        | Y         | Z         |
|----|----------|-----------|-----------|
| 7  | 1.826772 | -0.112334 | 0.697633  |
| 1  | 2.468552 | -0.912458 | 0.479206  |
| 1  | 2.430855 | 0.741149  | 0.594969  |
| 1  | 0.967775 | -0.085605 | 0.030783  |
| 1  | 1.498853 | -0.187599 | 1.658585  |
| 7  | 6.592120 | 0.113550  | -0.346623 |
| 1  | 7.112811 | -0.332414 | 0.405269  |
| 1  | 6.833990 | -0.389410 | -1.197487 |
| 1  | 6.999448 | 1.040364  | -0.451829 |
| 7  | 3.869927 | 1.863109  | 0.303773  |
| 1  | 3.743764 | 2.491343  | -0.485433 |
| 1  | 4.679278 | 1.273734  | 0.096426  |
| 1  | 4.115773 | 2.444671  | 1.100559  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 3.987039  | -1.892612 | 0.032842  |
| 1 | 4.279928  | -2.564685 | 0.737007  |
| 1 | 3.903048  | -2.405377 | -0.840809 |
| 1 | 4.746530  | -1.218669 | -0.080782 |
| 7 | -2.815985 | -0.081556 | 0.876264  |
| 1 | -2.882422 | 0.665528  | 1.562372  |
| 1 | -3.611895 | 0.036581  | 0.233339  |
| 1 | -2.977477 | -0.947423 | 1.383745  |
| 7 | -5.193615 | 0.275549  | -1.063804 |
| 1 | -5.230693 | 1.200615  | -1.482666 |
| 1 | -6.075839 | 0.141991  | -0.559974 |
| 1 | -5.190504 | -0.387317 | -1.833944 |
| 7 | -0.406904 | -0.048265 | -0.908152 |
| 1 | -1.237903 | -0.061251 | -0.286891 |
| 1 | -0.486367 | 0.783381  | -1.488718 |
| 1 | -0.496655 | -0.842710 | -1.537261 |
| 7 | -7.959312 | -0.117751 | 0.431833  |
| 1 | -8.116041 | -1.076093 | 0.729372  |
| 1 | -8.724517 | 0.127202  | -0.189649 |
| 1 | -8.050595 | 0.466630  | 1.257438  |

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Cartesian coordinates of : BL8\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.793432  | -0.734427 | -1.329992 |
| 1  | -0.681683 | -0.841511 | -0.563070 |
| 1  | 0.775642  | -0.161839 | -2.170726 |
| 1  | 1.482669  | -0.299321 | -0.681923 |
| 1  | 1.178519  | -1.633911 | -1.608660 |
| 7  | 2.765646  | 0.497920  | 0.514465  |
| 1  | 2.403624  | 1.017424  | 1.309537  |
| 1  | 3.399027  | -0.210775 | 0.895018  |
| 1  | 3.336836  | 1.155489  | -0.024183 |
| 7  | -1.623619 | -0.894199 | -0.020512 |
| 1  | -2.259071 | -0.088516 | -0.300880 |
| 1  | -2.096563 | -1.805988 | -0.204329 |
| 1  | -1.427088 | -0.823364 | 0.976288  |
| 7  | 4.597402  | 2.567644  | -1.113246 |
| 1  | 5.284264  | 2.938501  | -0.463202 |
| 1  | 5.114530  | 2.120713  | -1.864514 |
| 1  | 4.117259  | 3.364921  | -1.519686 |
| 7  | -2.943743 | -3.485038 | -0.539589 |
| 1  | -2.958755 | -3.705188 | -1.532263 |
| 1  | -3.910438 | -3.507706 | -0.224991 |
| 1  | -2.473344 | -4.260727 | -0.080116 |
| 7  | -3.296287 | 1.273259  | -0.762202 |
| 1  | -3.892989 | 1.606190  | 0.006886  |
| 1  | -2.746055 | 2.071393  | -1.070609 |
| 1  | -3.916481 | 1.043054  | -1.534892 |
| 7  | -5.136318 | 2.381907  | 1.486534  |
| 1  | -5.771524 | 1.707865  | 1.904535  |
| 1  | -4.635893 | 2.823328  | 2.252945  |
| 1  | -5.716273 | 3.103540  | 1.066835  |
| 7  | 4.846396  | -1.621844 | 1.734635  |
| 1  | 5.434937  | -1.099250 | 2.376856  |
| 1  | 4.481539  | -2.416511 | 2.251046  |
| 1  | 5.456949  | -1.994367 | 1.013451  |

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Cartesian coordinates of : BDC8\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z        |
|----|-----------|-----------|----------|
| 7  | -0.635321 | 0.024860  | 0.450435 |
| 1  | -0.279214 | -0.904451 | 0.076104 |
| 1  | -0.412587 | 0.076481  | 1.443651 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.159981 | 0.833227  | -0.031367 |
| 1 | -1.678223 | 0.089185  | 0.345055  |
| 7 | 2.699613  | -0.390335 | -0.756602 |
| 1 | 3.532439  | -0.301886 | -0.163270 |
| 1 | 3.034216  | -0.615282 | -1.690299 |
| 1 | 2.178875  | -1.202771 | -0.435702 |
| 7 | -3.485727 | 0.542249  | 0.267166  |
| 1 | -4.126851 | 0.411436  | 1.046151  |
| 1 | -4.026503 | 0.389669  | -0.580958 |
| 1 | -3.209437 | 1.533546  | 0.268894  |
| 7 | -2.042370 | 3.235794  | 0.195320  |
| 1 | -2.456801 | 3.859371  | -0.492280 |
| 1 | -1.995084 | 3.758871  | 1.065324  |
| 1 | -1.086224 | 3.052879  | -0.103029 |
| 7 | 0.040262  | -2.575328 | -0.438507 |
| 1 | 0.269759  | -2.725525 | -1.417882 |
| 1 | 0.636864  | -3.198359 | 0.100339  |
| 1 | -0.930591 | -2.886729 | -0.298564 |
| 7 | 0.956949  | 2.064919  | -0.798950 |
| 1 | 1.680245  | 1.328963  | -0.858482 |
| 1 | 1.376015  | 2.849225  | -0.304588 |
| 1 | 0.777779  | 2.384297  | -1.748138 |
| 7 | -2.935502 | -2.810464 | 0.165616  |
| 1 | -3.487174 | -3.221631 | -0.582410 |
| 1 | -3.178827 | -3.313747 | 1.014208  |
| 1 | -3.250353 | -1.849375 | 0.280230  |
| 7 | 5.357182  | -0.108553 | 0.897787  |
| 1 | 5.288505  | 0.015460  | 1.903760  |
| 1 | 5.935173  | -0.930314 | 0.745082  |
| 1 | 5.882370  | 0.685469  | 0.542317  |

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Cartesian coordinates of : DC8\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.134394 | 2.511611  | -1.042549 |
| 1  | -0.644975 | 1.850322  | -0.298559 |
| 1  | -0.197413 | 2.092983  | -1.969049 |
| 1  | -0.588955 | 3.422571  | -1.075221 |
| 1  | 0.920322  | 2.633984  | -0.771618 |
| 7  | -1.299214 | 0.878038  | 0.757127  |
| 1  | -2.272188 | 0.630076  | 0.555105  |
| 1  | -0.752846 | 0.003249  | 0.775352  |
| 1  | -1.283750 | 1.258566  | 1.700883  |
| 7  | 0.195293  | -1.786224 | 0.582153  |
| 1  | -0.590262 | -2.054335 | -0.017859 |
| 1  | 1.064442  | -1.952587 | 0.075811  |
| 1  | 0.194189  | -2.420144 | 1.376935  |
| 7  | 2.669430  | 0.085888  | 1.169096  |
| 1  | 3.300574  | 0.089226  | 1.965570  |
| 1  | 1.743988  | -0.163562 | 1.512081  |
| 1  | 2.944635  | -0.690450 | 0.565232  |
| 7  | 3.225478  | -2.603215 | -0.647963 |
| 1  | 2.777080  | -3.012181 | -1.463844 |
| 1  | 3.371968  | -3.364236 | 0.010505  |
| 1  | 4.149836  | -2.308982 | -0.953551 |
| 7  | -2.555382 | -2.029289 | -0.901446 |
| 1  | -3.102918 | -1.235496 | -0.573500 |
| 1  | -2.611211 | -2.042614 | -1.915478 |
| 1  | -3.019221 | -2.872126 | -0.574246 |
| 7  | -4.489391 | 0.361293  | 0.399811  |
| 1  | -4.692425 | 1.294439  | 0.750572  |
| 1  | -5.089447 | 0.233708  | -0.411740 |
| 1  | -4.828008 | -0.284346 | 1.109471  |
| 7  | 2.486207  | 2.703269  | -0.297357 |
| 1  | 2.706189  | 3.471795  | 0.331664  |
| 1  | 2.650990  | 1.820749  | 0.218347  |
| 1  | 3.163205  | 2.749804  | -1.054966 |

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Cartesian coordinates of : L8

| -----                                        |           |           |           |
|----------------------------------------------|-----------|-----------|-----------|
| Atomic number (AN) and Cartesian coordinates |           |           |           |
| AN                                           | X         | Y         | Z         |
| -----                                        |           |           |           |
| 7                                            | -1.154765 | -0.777049 | -0.006648 |
| 1                                            | -0.261904 | -0.120218 | 0.075887  |
| 1                                            | -1.254044 | -1.324663 | 0.846949  |
| 1                                            | -2.071948 | -0.197141 | -0.170685 |
| 1                                            | -1.021868 | -1.426854 | -0.780271 |
| 7                                            | -3.461933 | 0.638439  | -0.395139 |
| 1                                            | -3.632756 | 0.878406  | -1.369237 |
| 1                                            | -4.277083 | 0.082080  | -0.074902 |
| 1                                            | -3.482382 | 1.515910  | 0.119859  |
| 7                                            | 1.050731  | 0.781420  | 0.178684  |
| 1                                            | 1.178975  | 1.208084  | 1.093791  |
| 1                                            | 1.895525  | 0.201066  | -0.004495 |
| 1                                            | 1.064877  | 1.545077  | -0.494007 |
| 7                                            | 5.818300  | 1.025740  | 0.384639  |
| 1                                            | 5.829678  | 1.883716  | -0.159800 |
| 1                                            | 5.832933  | 1.306930  | 1.361056  |
| 1                                            | 6.705312  | 0.546160  | 0.201062  |
| 7                                            | 3.478706  | -0.846966 | -0.330289 |
| 1                                            | 4.264540  | -0.224451 | -0.091288 |
| 1                                            | 3.619408  | -1.135911 | -1.294818 |
| 1                                            | 3.588961  | -1.685005 | 0.234545  |
| 7                                            | -8.486462 | 0.531496  | -0.204151 |
| 1                                            | -9.257974 | 0.031369  | 0.228502  |
| 1                                            | -8.535914 | 1.489605  | 0.129918  |
| 1                                            | -8.679395 | 0.558787  | -1.201209 |
| 7                                            | -5.824446 | -0.967134 | 0.531590  |
| 1                                            | -5.905667 | -1.889282 | 0.111419  |
| 1                                            | -5.863738 | -1.110215 | 1.537355  |
| 1                                            | -6.675509 | -0.452975 | 0.275909  |
| 7                                            | 8.597625  | -0.391138 | -0.151235 |
| 1                                            | 8.729902  | -1.228977 | 0.407436  |
| 1                                            | 9.353794  | 0.244155  | 0.086458  |
| 1                                            | 8.731985  | -0.659302 | -1.121587 |
| -----                                        |           |           |           |

Cartesian coordinates of the protonated ammonia nanomer

Cartesian coordinates of : TC9\_1

| -----                                        |           |           |           |
|----------------------------------------------|-----------|-----------|-----------|
| Atomic number (AN) and Cartesian coordinates |           |           |           |
| AN                                           | X         | Y         | Z         |
| -----                                        |           |           |           |
| 7                                            | -0.726290 | -0.007867 | 0.262037  |
| 1                                            | 0.068420  | -0.005185 | -0.427513 |
| 1                                            | -1.346588 | 0.814274  | 0.122349  |
| 1                                            | -1.343114 | -0.831130 | 0.119163  |
| 1                                            | -0.323165 | -0.008997 | 1.236287  |
| 7                                            | 0.632562  | -0.008747 | 2.774931  |
| 1                                            | 0.543636  | -0.824848 | 3.373613  |
| 1                                            | 0.537435  | 0.804355  | 3.376735  |
| 1                                            | 1.585103  | -0.004378 | 2.387547  |
| 7                                            | -2.953069 | -1.887067 | -0.188321 |
| 1                                            | -3.181131 | -2.524172 | 0.569776  |
| 1                                            | -2.941844 | -2.439609 | -1.040978 |
| 1                                            | -3.722919 | -1.220925 | -0.268067 |
| 7                                            | -5.654404 | 0.009704  | -0.402893 |
| 1                                            | -6.079660 | 0.891102  | -0.681530 |
| 1                                            | -6.005940 | -0.685128 | -1.057598 |
| 1                                            | -6.056194 | -0.222280 | 0.502381  |
| 7                                            | 3.417574  | 2.621055  | -0.911759 |
| 1                                            | 4.408538  | 2.488093  | -1.097315 |
| 1                                            | 3.353349  | 3.254601  | -0.118926 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.045997  | 3.130413  | -1.709746 |
| 7 | -2.941098 | 1.883160  | -0.174395 |
| 1 | -2.922051 | 2.444372  | -1.021312 |
| 1 | -3.156522 | 2.516515  | 0.590612  |
| 1 | -3.724287 | 1.232852  | -0.259515 |
| 7 | 1.549351  | -0.000527 | -1.518375 |
| 1 | 1.348506  | -0.000769 | -2.514747 |
| 1 | 2.123737  | 0.823817  | -1.328477 |
| 1 | 2.128780  | -0.821474 | -1.329078 |
| 7 | 3.258915  | 0.003574  | 1.169420  |
| 1 | 3.280336  | -0.813987 | 0.561183  |
| 1 | 3.274394  | 0.822161  | 0.562382  |
| 1 | 4.122850  | 0.006330  | 1.704153  |
| 7 | 3.433696  | -2.611208 | -0.913516 |
| 1 | 3.371004  | -3.245978 | -0.121540 |
| 1 | 4.424357  | -2.473087 | -1.096900 |
| 1 | 3.066310  | -3.121477 | -1.712862 |

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Cartesian coordinates of : BTC9\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.622664 | 1.485256  | 0.051484  |
| 1  | -0.486003 | 0.908228  | 0.911642  |
| 1  | -0.726277 | 2.490716  | 0.286193  |
| 1  | 0.208533  | 1.315127  | -0.567189 |
| 1  | -1.466226 | 1.130844  | -0.462451 |
| 7  | -2.729979 | 0.233715  | -1.461359 |
| 1  | -3.111336 | -0.526117 | -0.894998 |
| 1  | -2.179593 | -0.203738 | -2.196659 |
| 1  | -3.505365 | 0.718119  | -1.903792 |
| 7  | -0.048534 | -0.329138 | 2.264656  |
| 1  | 0.256718  | 0.093111  | 3.137395  |
| 1  | -0.795258 | -0.975873 | 2.504442  |
| 1  | 0.731803  | -0.884270 | 1.902127  |
| 7  | 2.391684  | -1.944147 | 0.955192  |
| 1  | 2.973190  | -1.248580 | 0.482190  |
| 1  | 2.462465  | -2.798099 | 0.406543  |
| 1  | 2.846748  | -2.150715 | 1.841462  |
| 7  | -0.441201 | -1.855617 | -0.697851 |
| 1  | -0.463635 | -2.744954 | -1.190127 |
| 1  | -1.352166 | -1.748976 | -0.253213 |
| 1  | 0.262894  | -1.936708 | 0.035814  |
| 7  | -0.954647 | 4.389091  | 0.687098  |
| 1  | -0.402673 | 4.700593  | 1.481834  |
| 1  | -0.683164 | 4.972294  | -0.100140 |
| 1  | -1.921824 | 4.620494  | 0.898199  |
| 7  | 1.446128  | 0.461781  | -1.623469 |
| 1  | 0.894908  | -0.398690 | -1.666717 |
| 1  | 2.337697  | 0.240456  | -1.181548 |
| 1  | 1.640072  | 0.768905  | -2.571778 |
| 7  | 4.535005  | 0.034662  | -0.508683 |
| 1  | 5.224651  | -0.285099 | 0.167335  |
| 1  | 4.604717  | 1.049257  | -0.521665 |
| 1  | 4.860290  | -0.289391 | -1.416302 |
| 7  | -3.649231 | -2.333489 | 0.280378  |
| 1  | -4.417005 | -1.928240 | 0.810325  |
| 1  | -3.205648 | -3.008979 | 0.897824  |
| 1  | -4.074439 | -2.874518 | -0.468873 |

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Cartesian coordinates of : TC9\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z        |
|----|-----------|-----------|----------|
| 7  | -1.189644 | -0.264188 | 0.678725 |
| 1  | -0.210180 | 0.074804  | 0.847915 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.751488 | 0.451453  | 0.153576  |
| 1 | -1.072103 | -1.132631 | 0.103675  |
| 1 | -1.653174 | -0.489132 | 1.579301  |
| 7 | -5.545877 | 0.737077  | -1.789999 |
| 1 | -5.745677 | 1.219926  | -2.661633 |
| 1 | -5.636459 | -0.256697 | -1.980519 |
| 1 | -6.293855 | 0.980233  | -1.146662 |
| 7 | 1.640431  | 0.180788  | 0.904681  |
| 1 | 1.949547  | -0.528699 | 0.237160  |
| 1 | 2.106048  | 1.052109  | 0.645211  |
| 1 | 2.024582  | -0.088937 | 1.806929  |
| 7 | 4.705619  | 0.193297  | -0.568760 |
| 1 | 5.274624  | 0.447050  | -1.371339 |
| 1 | 4.196829  | 1.026391  | -0.275795 |
| 1 | 5.348910  | -0.047240 | 0.180057  |
| 7 | 3.213444  | 3.023503  | 0.335221  |
| 1 | 3.305396  | 3.430606  | -0.592069 |
| 1 | 4.052834  | 3.281716  | 0.848190  |
| 1 | 2.445096  | 3.514107  | 0.785924  |
| 7 | 2.777942  | -2.177692 | -1.172269 |
| 1 | 3.147852  | -3.007973 | -0.715600 |
| 1 | 2.775427  | -2.384865 | -2.168283 |
| 1 | 3.472189  | -1.433425 | -1.033068 |
| 7 | -0.365452 | -2.549266 | -0.881207 |
| 1 | 0.646288  | -2.386576 | -0.933313 |
| 1 | -0.501363 | -3.470042 | -0.472856 |
| 1 | -0.709866 | -2.604546 | -1.835893 |
| 7 | -2.744993 | 1.703147  | -0.777601 |
| 1 | -3.656158 | 1.342032  | -1.085483 |
| 1 | -2.932820 | 2.539282  | -0.230202 |
| 1 | -2.258509 | 2.016171  | -1.613961 |
| 7 | -2.524626 | -0.921528 | 3.282662  |
| 1 | -2.502374 | -0.144730 | 3.938007  |
| 1 | -2.086369 | -1.709215 | 3.752650  |
| 1 | -3.503131 | -1.167142 | 3.157912  |

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Cartesian coordinates of : BL9\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.000002 | 0.000073  | 0.000018  |
| 1  | -0.643510 | -0.561102 | 0.606561  |
| 1  | 0.561169  | -0.643429 | -0.606534 |
| 1  | -0.561169 | 0.643585  | -0.606530 |
| 1  | 0.643499  | 0.561241  | 0.606575  |
| 7  | -1.540299 | 1.775414  | -1.741031 |
| 1  | -2.071935 | 1.248274  | -2.429059 |
| 1  | -2.210958 | 2.376262  | -1.248157 |
| 1  | -0.928732 | 2.392838  | -2.268890 |
| 7  | -1.775294 | -1.540273 | 1.741073  |
| 1  | -2.392404 | -0.928693 | 2.269282  |
| 1  | -2.376460 | -2.210622 | 1.248163  |
| 1  | -1.248113 | -2.072261 | 2.428797  |
| 7  | 1.775256  | 1.540419  | 1.741108  |
| 1  | 2.376538  | 2.210657  | 1.248189  |
| 1  | 2.392252  | 0.928837  | 2.269450  |
| 1  | 1.248051  | 2.072531  | 2.428718  |
| 7  | -3.641707 | 3.686591  | -0.396624 |
| 1  | -3.288729 | 4.247991  | 0.372925  |
| 1  | -4.470248 | 3.208881  | -0.053976 |
| 1  | -3.955548 | 4.336426  | -1.112088 |
| 7  | 3.687654  | 3.640632  | 0.396569  |
| 1  | 3.210350  | 4.469258  | 0.053563  |
| 1  | 4.337438  | 3.954429  | 1.112098  |
| 1  | 4.249102  | 3.287210  | -0.372742 |
| 7  | 1.540301  | -1.775238 | -1.741054 |
| 1  | 0.928721  | -2.392542 | -2.269038 |
| 1  | 2.072060  | -1.248083 | -2.428974 |
| 1  | 2.210849  | -2.376208 | -1.248177 |

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7      -3.687324      -3.640860      0.396592
1      -4.337622      -3.954086      1.111905
1      -4.248215      -3.287865      -0.373320
1      -3.209921      -4.469786      0.054449
7      3.641414      -3.686742      -0.396647
1      3.954957      -4.336806      -1.112034
1      3.288462      -4.247891      0.373097
1      4.470136      -3.209151      -0.054272

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Cartesian coordinates of :     BDC9\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.090109 | -0.086855 | -0.046448 |
| 1  | 0.681443  | -0.214596 | 0.641973  |
| 1  | -0.335200 | -0.979793 | -0.521692 |
| 1  | -0.979716 | 0.223431  | 0.423418  |
| 1  | 0.262154  | 0.626168  | -0.725896 |
| 7  | 1.330972  | 1.863367  | -1.651542 |
| 1  | 1.078401  | 2.836957  | -1.505392 |
| 1  | 1.358434  | 1.722659  | -2.657811 |
| 1  | 2.287792  | 1.740870  | -1.302105 |
| 7  | -2.696510 | 0.312142  | 1.051537  |
| 1  | -3.222368 | 1.156420  | 0.800516  |
| 1  | -2.768993 | 0.207554  | 2.060013  |
| 1  | -3.171785 | -0.488172 | 0.634422  |
| 7  | -4.474921 | -2.262339 | -0.212488 |
| 1  | -4.651579 | -3.108258 | -0.749315 |
| 1  | -4.782169 | -2.462982 | 0.736038  |
| 1  | -5.110830 | -1.558507 | -0.579354 |
| 7  | 4.977678  | -1.649922 | 0.658191  |
| 1  | 5.840419  | -1.346185 | 1.103074  |
| 1  | 5.237182  | -2.011156 | -0.256418 |
| 1  | 4.651575  | -2.451665 | 1.192594  |
| 7  | -1.358245 | -2.480967 | -1.155673 |
| 1  | -1.039390 | -3.383308 | -0.813800 |
| 1  | -1.403514 | -2.553799 | -2.168350 |
| 1  | -2.315406 | -2.351338 | -0.818756 |
| 7  | 2.326441  | 0.069683  | 1.577678  |
| 1  | 2.299384  | 0.047794  | 2.593163  |
| 1  | 3.098461  | -0.527947 | 1.277604  |
| 1  | 2.582249  | 1.015153  | 1.300999  |
| 7  | 4.290095  | 1.333787  | -0.633652 |
| 1  | 4.754568  | 1.997604  | -0.019422 |
| 1  | 4.462899  | 0.402090  | -0.255180 |
| 1  | 4.774662  | 1.389197  | -1.525770 |
| 7  | -4.315338 | 2.939529  | 0.417497  |
| 1  | -5.233061 | 2.920386  | 0.853188  |
| 1  | -4.462947 | 3.146698  | -0.566035 |
| 1  | -3.823106 | 3.735757  | 0.812586  |

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Cartesian coordinates of :     BTC9\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.124377 | 0.819093  | -0.029345 |
| 1  | -1.940099 | 0.358646  | 0.889114  |
| 1  | -2.614643 | 1.729429  | 0.070520  |
| 1  | -1.185712 | 0.902442  | -0.481119 |
| 1  | -2.660726 | 0.140994  | -0.625327 |
| 7  | -3.047819 | -1.333332 | -1.657757 |
| 1  | -3.888931 | -1.858599 | -1.436370 |
| 1  | -2.241449 | -1.924999 | -1.434552 |
| 1  | -3.055457 | -1.181832 | -2.662473 |
| 7  | -1.167973 | -0.775814 | 2.197707  |
| 1  | -0.917619 | -0.336245 | 3.079290  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.755736 | -1.572457 | 2.428250  |
| 1 | -0.307143 | -1.144198 | 1.787673  |
| 7 | 1.783991  | -1.802281 | 1.228280  |
| 1 | 2.100070  | -0.828679 | 1.176082  |
| 1 | 2.416825  | -2.333035 | 0.633220  |
| 1 | 1.964899  | -2.126790 | 2.175556  |
| 7 | -0.571158 | -3.017056 | -0.577207 |
| 1 | -0.063509 | -3.508004 | -1.309340 |
| 1 | -1.142341 | -3.721732 | -0.116744 |
| 1 | 0.121510  | -2.703595 | 0.107281  |
| 7 | -3.590358 | 3.392510  | 0.224679  |
| 1 | -3.411372 | 3.884742  | 1.095995  |
| 1 | -3.368649 | 4.042151  | -0.525333 |
| 1 | -4.594180 | 3.235864  | 0.182988  |
| 7 | 0.455108  | 0.214278  | -1.106197 |
| 1 | 0.245115  | -0.783624 | -1.100287 |
| 1 | 1.230640  | 0.367065  | -0.459638 |
| 1 | 0.781736  | 0.453116  | -2.037994 |
| 7 | 2.840638  | 1.184304  | 0.888587  |
| 1 | 3.312067  | 1.170550  | 1.790373  |
| 1 | 2.351244  | 2.075408  | 0.851123  |
| 1 | 3.583367  | 1.225711  | 0.180434  |
| 7 | 5.205832  | 1.355141  | -1.177682 |
| 1 | 5.609430  | 2.285790  | -1.116082 |
| 1 | 5.001944  | 1.191057  | -2.159273 |
| 1 | 5.941529  | 0.702910  | -0.920828 |

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Cartesian coordinates of : BTC9\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.743103  | 0.285620  | -0.384490 |
| 1  | 1.422043  | -0.428168 | -1.071016 |
| 1  | 2.419536  | 0.957091  | -0.793219 |
| 1  | 0.862075  | 0.747328  | -0.036302 |
| 1  | 2.161631  | -0.259656 | 0.408911  |
| 7  | 2.464715  | -1.564570 | 1.681201  |
| 1  | 3.246932  | -2.189192 | 1.505847  |
| 1  | 1.603148  | -2.119296 | 1.625810  |
| 1  | 2.561785  | -1.243177 | 2.640326  |
| 7  | 0.416745  | -1.969627 | -1.603386 |
| 1  | 0.325550  | -2.260533 | -2.572223 |
| 1  | 0.815193  | -2.750810 | -1.088177 |
| 1  | -0.521813 | -1.823591 | -1.227680 |
| 7  | -2.633890 | -1.576044 | -0.418419 |
| 1  | -2.720423 | -0.718218 | -0.970341 |
| 1  | -3.235554 | -1.452221 | 0.393127  |
| 1  | -3.058509 | -2.323424 | -0.963043 |
| 7  | -0.324414 | -3.017961 | 1.399338  |
| 1  | -0.662923 | -3.018103 | 2.358301  |
| 1  | -0.296004 | -3.994167 | 1.115707  |
| 1  | -1.038784 | -2.561469 | 0.828791  |
| 7  | 3.765638  | 2.161292  | -1.533664 |
| 1  | 3.921446  | 2.012733  | -2.527213 |
| 1  | 3.528929  | 3.143424  | -1.421066 |
| 1  | 4.664313  | 2.026716  | -1.077529 |
| 7  | -0.852781 | 1.016940  | 0.527343  |
| 1  | -1.079897 | 0.171283  | 1.046216  |
| 1  | -1.506068 | 1.047280  | -0.254690 |
| 1  | -1.047379 | 1.818323  | 1.137294  |
| 7  | -2.956218 | 1.162386  | -2.108751 |
| 1  | -3.562578 | 0.735060  | -2.804827 |
| 1  | -2.220527 | 1.635048  | -2.627657 |
| 1  | -3.509882 | 1.889427  | -1.662376 |
| 7  | -1.424666 | 3.459776  | 2.439560  |
| 1  | -1.383043 | 4.361950  | 1.974084  |
| 1  | -0.739470 | 3.488760  | 3.189311  |
| 1  | -2.337352 | 3.402913  | 2.882512  |

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Cartesian coordinates of : BC9\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.015715  | -0.455034 | 0.698628  |
| 1  | 0.159060  | -1.027946 | 0.872109  |
| 1  | 0.682505  | 0.329519  | 0.075216  |
| 1  | 1.388921  | -0.086662 | 1.592718  |
| 1  | 1.746833  | -1.032574 | 0.214679  |
| 7  | -0.515150 | 4.489818  | -0.333762 |
| 1  | -1.017913 | 4.745213  | 0.511184  |
| 1  | -0.987184 | 4.952740  | -1.105335 |
| 1  | 0.407378  | 4.909430  | -0.263293 |
| 7  | 3.004326  | -2.107051 | -0.625537 |
| 1  | 3.337324  | -2.849470 | -0.015505 |
| 1  | 2.609134  | -2.568655 | -1.440987 |
| 1  | 3.835099  | -1.598289 | -0.950587 |
| 7  | -3.436166 | 0.228267  | -0.970408 |
| 1  | -3.407196 | 0.255956  | -1.986896 |
| 1  | -4.190292 | -0.423162 | -0.722563 |
| 1  | -3.745340 | 1.150131  | -0.671407 |
| 7  | -1.614777 | -1.683628 | 0.837596  |
| 1  | -2.151145 | -1.042009 | 0.244951  |
| 1  | -2.079002 | -1.712883 | 1.741209  |
| 1  | -1.710114 | -2.611844 | 0.434764  |
| 7  | -0.333426 | 1.397375  | -0.980634 |
| 1  | -0.398531 | 2.385893  | -0.716416 |
| 1  | -0.061465 | 1.372975  | -1.959809 |
| 1  | -1.270924 | 0.995448  | -0.922881 |
| 7  | -5.747637 | -1.771315 | -0.225591 |
| 1  | -5.963255 | -1.821144 | 0.765938  |
| 1  | -6.591500 | -1.448146 | -0.690634 |
| 1  | -5.589782 | -2.724533 | -0.539577 |
| 7  | 5.598330  | -0.712915 | -1.698116 |
| 1  | 5.426771  | 0.007315  | -2.393769 |
| 1  | 6.191573  | -0.296398 | -0.986332 |
| 1  | 6.152630  | -1.432367 | -2.154078 |
| 7  | 2.100922  | 0.550297  | 3.314408  |
| 1  | 1.502592  | 1.250010  | 3.745072  |
| 1  | 3.019628  | 0.973922  | 3.216487  |
| 1  | 2.199243  | -0.203174 | 3.989647  |

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Cartesian coordinates of : BDC9\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.676878  | 0.247290  | 0.020988  |
| 1  | 2.317609  | 0.208336  | 0.840122  |
| 1  | 2.271120  | 0.001379  | -0.798857 |
| 1  | 0.868503  | -0.410360 | 0.127825  |
| 1  | 1.240656  | 1.194818  | -0.085376 |
| 7  | 6.517668  | -0.762959 | -0.027516 |
| 1  | 7.036566  | 0.054194  | 0.285460  |
| 1  | 6.755157  | -1.515561 | 0.614518  |
| 1  | 6.925006  | -1.024579 | -0.922594 |
| 7  | 3.783813  | -0.479921 | -1.864992 |
| 1  | 3.687239  | -1.373447 | -2.339539 |
| 1  | 4.586123  | -0.555145 | -1.236720 |
| 1  | 4.021320  | 0.204327  | -2.577948 |
| 7  | 3.918761  | -0.013308 | 1.882694  |
| 1  | 4.210532  | 0.819747  | 2.386261  |
| 1  | 3.871907  | -0.765195 | 2.564721  |
| 1  | 4.661715  | -0.246625 | 1.222077  |
| 7  | -2.957557 | 1.379666  | -0.056445 |
| 1  | -3.259530 | 1.906611  | -0.872865 |
| 1  | -3.506867 | 0.508198  | -0.059579 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -3.272008 | 1.912184  | 0.751498  |
| 7 | -4.504641 | -1.290326 | -0.062686 |
| 1 | -4.385150 | -1.850525 | -0.902379 |
| 1 | -5.496192 | -1.029934 | -0.022861 |
| 1 | -4.335105 | -1.911860 | 0.723391  |
| 7 | -0.862325 | -1.088465 | 0.271587  |
| 1 | -1.489697 | -0.287472 | 0.160967  |
| 1 | -1.130408 | -1.765522 | -0.437698 |
| 1 | -1.084657 | -1.511556 | 1.168795  |
| 7 | -7.561228 | -0.526278 | 0.052912  |
| 1 | -7.813478 | -0.026724 | 0.900633  |
| 1 | -8.134721 | -1.364362 | 0.024188  |
| 1 | -7.851288 | 0.054932  | -0.728020 |
| 7 | 0.006475  | 2.575058  | -0.222712 |
| 1 | 0.036712  | 3.085505  | -1.101099 |
| 1 | 0.060727  | 3.269701  | 0.517274  |
| 1 | -0.916697 | 2.133634  | -0.159011 |

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Cartesian coordinates of : BDC9\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.933782  | 1.189689  | 0.266104  |
| 1  | 1.140576  | 0.392775  | -0.422119 |
| 1  | 1.543172  | 1.105262  | 1.099748  |
| 1  | 1.111124  | 2.102373  | -0.191287 |
| 1  | -0.075201 | 1.124190  | 0.552021  |
| 7  | -3.768351 | 0.872452  | -1.681169 |
| 1  | -4.597869 | 0.294267  | -1.573322 |
| 1  | -3.480812 | 0.788704  | -2.652902 |
| 1  | -4.075451 | 1.834229  | -1.559238 |
| 7  | -1.720458 | -1.659158 | -0.859357 |
| 1  | -2.104038 | -2.491141 | -1.298420 |
| 1  | -1.841333 | -1.762493 | 0.146865  |
| 1  | -2.298126 | -0.869699 | -1.144404 |
| 7  | 1.247789  | -0.933977 | -1.512967 |
| 1  | 0.315564  | -1.346581 | -1.397394 |
| 1  | 1.344717  | -0.678038 | -2.491913 |
| 1  | 1.951500  | -1.655211 | -1.328177 |
| 7  | 1.513066  | 3.830423  | -1.073203 |
| 1  | 1.244686  | 4.636703  | -0.515508 |
| 1  | 1.031940  | 3.920579  | -1.964005 |
| 1  | 2.505392  | 3.930705  | -1.269645 |
| 7  | -2.467979 | -1.956374 | 2.409566  |
| 1  | -3.391740 | -2.311316 | 2.175667  |
| 1  | -1.856781 | -2.765416 | 2.485129  |
| 1  | -2.541671 | -1.569004 | 3.346937  |
| 7  | 2.760370  | 0.977159  | 2.655564  |
| 1  | 3.733859  | 0.964527  | 2.363373  |
| 1  | 2.605498  | 0.123449  | 3.184807  |
| 1  | 2.663472  | 1.747551  | 3.311444  |
| 7  | -1.866698 | 0.927542  | 0.988865  |
| 1  | -2.237918 | 1.647621  | 1.602722  |
| 1  | -2.022668 | 0.029429  | 1.452095  |
| 1  | -2.439985 | 0.930712  | 0.142261  |
| 7  | 3.458949  | -3.200544 | -1.234697 |
| 1  | 4.396408  | -2.860920 | -1.428900 |
| 1  | 3.231145  | -3.865565 | -1.968360 |
| 1  | 3.511240  | -3.728171 | -0.368427 |

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Cartesian coordinates of : BDC9\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.848522 | -2.038838 | -1.994969 |
| 1  | -0.577382 | -1.819449 | -0.663151 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -2.458333 | -2.846623 | -1.903460 |
| 1 | -2.431618 | -1.199784 | -1.890840 |
| 1 | -1.497875 | -2.051291 | -2.948702 |
| 7 | 0.015478  | -1.433250 | 0.111221  |
| 1 | -0.181418 | -1.935163 | 0.995986  |
| 1 | 1.027535  | -1.506291 | -0.123588 |
| 1 | -0.244609 | -0.404744 | 0.182506  |
| 7 | 4.917111  | 1.018626  | -0.576561 |
| 1 | 5.318228  | 1.514883  | 0.215541  |
| 1 | 4.879903  | 1.684420  | -1.344591 |
| 1 | 5.604194  | 0.318005  | -0.845185 |
| 7 | 2.182629  | 2.491591  | 0.621931  |
| 1 | 2.855665  | 1.816975  | 0.261859  |
| 1 | 2.377312  | 3.383384  | 0.176116  |
| 1 | 2.372891  | 2.610323  | 1.612571  |
| 7 | 2.899531  | -1.540926 | -0.563385 |
| 1 | 3.028405  | -1.867805 | -1.517516 |
| 1 | 3.415245  | -2.183886 | 0.031771  |
| 1 | 3.368699  | -0.635177 | -0.495622 |
| 7 | -0.635120 | 1.300895  | -0.020938 |
| 1 | -1.452724 | 1.658547  | 0.473266  |
| 1 | 0.193853  | 1.841065  | 0.247349  |
| 1 | -0.799247 | 1.467457  | -1.010715 |
| 7 | -3.444029 | 2.492118  | 1.210256  |
| 1 | -2.969448 | 2.876135  | 2.023747  |
| 1 | -3.765486 | 3.289432  | 0.666904  |
| 1 | -4.277908 | 2.029677  | 1.563554  |
| 7 | -3.584020 | 0.530299  | -1.475176 |
| 1 | -3.388038 | 1.014741  | -0.599257 |
| 1 | -4.545388 | 0.203568  | -1.427750 |
| 1 | -3.556254 | 1.226260  | -2.215400 |
| 7 | -0.558359 | -2.961960 | 2.639549  |
| 1 | -1.526409 | -2.861359 | 2.932695  |
| 1 | 0.014689  | -2.675924 | 3.428774  |
| 1 | -0.397370 | -3.957259 | 2.509638  |

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Cartesian coordinates of : BDC9\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.705775 | -0.211516 | -0.002776 |
| 1  | -1.587572 | -1.259652 | -0.012244 |
| 1  | -2.234216 | 0.083479  | -0.843926 |
| 1  | -2.231833 | 0.068613  | 0.844942  |
| 1  | -0.735225 | 0.231361  | -0.000175 |
| 7  | 2.646778  | -0.336447 | 2.602192  |
| 1  | 3.636499  | -0.240109 | 2.390221  |
| 1  | 2.560151  | -1.138302 | 3.221454  |
| 1  | 2.391214  | 0.477317  | 3.155517  |
| 7  | 1.846087  | -2.229053 | -0.007053 |
| 1  | 2.524655  | -2.985285 | -0.007958 |
| 1  | 2.037287  | -1.647461 | -0.822544 |
| 1  | 2.030728  | -1.655336 | 0.815503  |
| 7  | -1.117860 | -3.009604 | -0.028030 |
| 1  | -0.093829 | -2.907496 | -0.021283 |
| 1  | -1.380252 | -3.569173 | 0.778450  |
| 1  | -1.371129 | -3.550486 | -0.850042 |
| 7  | -3.305601 | 0.526983  | 2.443466  |
| 1  | -3.330407 | 1.523926  | 2.639596  |
| 1  | -2.942951 | 0.075650  | 3.278898  |
| 1  | -4.271867 | 0.225634  | 2.349005  |
| 7  | 2.663970  | -0.313003 | -2.593552 |
| 1  | 3.652841  | -0.224769 | -2.374184 |
| 1  | 2.576711  | -1.107523 | -3.222110 |
| 1  | 2.416866  | 0.508295  | -3.139536 |
| 7  | -3.311504 | 0.566765  | -2.432834 |
| 1  | -4.162915 | 0.014118  | -2.488820 |
| 1  | -2.803047 | 0.402488  | -3.297448 |
| 1  | -3.597414 | 1.542029  | -2.445291 |

|   |          |          |           |
|---|----------|----------|-----------|
| 7 | 0.917137 | 0.843193 | 0.004090  |
| 1 | 1.005794 | 1.863747 | 0.008163  |
| 1 | 1.418390 | 0.494235 | -0.814489 |
| 1 | 1.414832 | 0.487821 | 0.822072  |
| 7 | 1.248124 | 4.028519 | 0.013623  |
| 1 | 1.761011 | 4.342826 | 0.832403  |
| 1 | 0.370669 | 4.540277 | 0.005791  |
| 1 | 1.775520 | 4.342927 | -0.795855 |

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Cartesian coordinates of : BDC9\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.092953 | -0.000504 | 0.289583  |
| 1  | -1.516441 | -0.003907 | 1.176797  |
| 1  | -2.697382 | -0.843170 | 0.263110  |
| 1  | -2.690674 | 0.846968  | 0.265074  |
| 1  | -1.433783 | -0.002087 | -0.537953 |
| 7  | 1.763381  | 2.534532  | -1.803913 |
| 1  | 2.708379  | 2.260284  | -2.059998 |
| 1  | 1.850168  | 3.200255  | -1.040510 |
| 1  | 1.391921  | 3.054293  | -2.594914 |
| 7  | 1.910318  | -0.000324 | 0.471472  |
| 1  | 2.868225  | 0.001611  | 0.832523  |
| 1  | 1.805933  | -0.814368 | -0.131056 |
| 1  | 1.802591  | 0.813404  | -0.130891 |
| 7  | -0.331793 | -0.009952 | 2.520536  |
| 1  | 0.533657  | -0.006132 | 1.959648  |
| 1  | -0.313356 | 0.801067  | 3.132261  |
| 1  | -0.312119 | -0.828243 | 3.122478  |
| 7  | -3.858228 | 2.431366  | 0.268860  |
| 1  | -4.357840 | 2.560155  | -0.606955 |
| 1  | -3.332730 | 3.286203  | 0.431114  |
| 1  | -4.562681 | 2.382390  | 1.000177  |
| 7  | 1.770641  | -2.537790 | -1.801048 |
| 1  | 2.715237  | -2.260849 | -2.055733 |
| 1  | 1.858192  | -3.203142 | -1.037404 |
| 1  | 1.401972  | -3.058704 | -2.592597 |
| 7  | -3.876231 | -2.418747 | 0.266138  |
| 1  | -4.335093 | -2.542757 | 1.164791  |
| 1  | -3.364651 | -3.277485 | 0.081713  |
| 1  | -4.613870 | -2.365939 | -0.431275 |
| 7  | -0.252008 | -0.004259 | -1.905567 |
| 1  | -0.678188 | -0.005832 | -2.828545 |
| 1  | 0.355305  | -0.826573 | -1.855835 |
| 1  | 0.353642  | 0.819409  | -1.857762 |
| 7  | 4.834548  | 0.005122  | 1.760311  |
| 1  | 4.922832  | 0.820837  | 2.359391  |
| 1  | 5.643104  | 0.004601  | 1.145528  |
| 1  | 4.923921  | -0.808389 | 2.362219  |

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Cartesian coordinates of : BDC9\_7

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.238520 | -0.747997 | 0.600089  |
| 1  | -0.725583 | -1.272001 | 1.350375  |
| 1  | 0.244647  | -1.413430 | -0.045370 |
| 1  | -0.936049 | -0.140227 | 0.066239  |
| 1  | 0.526262  | -0.172861 | 1.008060  |
| 7  | -2.089706 | 0.838542  | -0.812303 |
| 1  | -2.762565 | 0.267719  | -1.334829 |
| 1  | -2.626350 | 1.462343  | -0.200605 |
| 1  | -1.629160 | 1.434424  | -1.495887 |
| 7  | -1.656046 | -2.278293 | 2.765201  |
| 1  | -1.478974 | -3.277904 | 2.714196  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.388343 | -1.983394 | 3.700341  |
| 1 | -2.663166 | -2.157856 | 2.699417  |
| 7 | 4.185037  | -0.623623 | -0.946845 |
| 1 | 4.486842  | -0.747391 | -1.909817 |
| 1 | 4.044555  | 0.376578  | -0.801270 |
| 1 | 4.972311  | -0.902998 | -0.367364 |
| 7 | -4.179432 | -0.824255 | -2.537367 |
| 1 | -4.527899 | -0.197334 | -3.257050 |
| 1 | -3.810277 | -1.641075 | -3.015145 |
| 1 | -4.987542 | -1.136008 | -2.006604 |
| 7 | 1.530108  | -2.361533 | -1.055569 |
| 1 | 2.406426  | -1.832176 | -0.989970 |
| 1 | 1.725576  | -3.307592 | -0.739620 |
| 1 | 1.296197  | -2.432406 | -2.042195 |
| 7 | 2.321475  | 0.396282  | 1.462880  |
| 1 | 2.871845  | -0.439350 | 1.276501  |
| 1 | 2.705745  | 1.122529  | 0.856547  |
| 1 | 2.505656  | 0.672776  | 2.423093  |
| 7 | -3.771632 | 2.872172  | 0.964906  |
| 1 | -3.287810 | 3.292775  | 1.752761  |
| 1 | -4.628792 | 2.467004  | 1.329691  |
| 1 | -4.047890 | 3.633234  | 0.351038  |
| 7 | 3.861418  | 2.635203  | -0.414656 |
| 1 | 3.860568  | 2.817342  | -1.415228 |
| 1 | 4.814835  | 2.788857  | -0.095503 |
| 1 | 3.300019  | 3.372934  | 0.003857  |

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Cartesian coordinates of : BL9\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.961342 | 0.026276  | 0.287600  |
| 1  | -0.799326 | -0.913440 | -0.151571 |
| 1  | -1.480700 | -0.088115 | 1.177307  |
| 1  | -0.026491 | 0.475534  | 0.480905  |
| 1  | -1.514627 | 0.628553  | -0.369525 |
| 7  | 1.619551  | 1.195546  | 0.782467  |
| 1  | 1.835447  | 1.315066  | 1.768919  |
| 1  | 2.358345  | 0.594536  | 0.388216  |
| 1  | 1.729635  | 2.112251  | 0.356347  |
| 7  | -0.388051 | -2.532878 | -0.961294 |
| 1  | 0.541268  | -2.829087 | -0.673370 |
| 1  | -1.025306 | -3.311823 | -0.758334 |
| 1  | -0.355095 | -2.439834 | -1.973365 |
| 7  | -2.473392 | 1.663279  | -1.587864 |
| 1  | -2.820591 | 2.549889  | -1.203469 |
| 1  | -3.282651 | 1.166793  | -1.952114 |
| 1  | -1.901746 | 1.900648  | -2.394754 |
| 7  | 3.892458  | -0.533561 | -0.371337 |
| 1  | 3.823060  | -0.732101 | -1.365599 |
| 1  | 4.038221  | -1.427066 | 0.090401  |
| 1  | 4.752297  | 0.009291  | -0.238297 |
| 7  | -3.598543 | 4.417620  | -0.591865 |
| 1  | -3.012854 | 4.937083  | 0.055504  |
| 1  | -3.714303 | 5.003170  | -1.414357 |
| 1  | -4.514853 | 4.340385  | -0.159767 |
| 7  | -2.440100 | -0.299958 | 2.889628  |
| 1  | -2.090173 | -1.088877 | 3.426549  |
| 1  | -2.351660 | 0.518879  | 3.485251  |
| 1  | -3.435517 | -0.456736 | 2.757042  |
| 7  | -2.251535 | -5.013557 | -0.489558 |
| 1  | -1.959317 | -5.726244 | -1.152484 |
| 1  | -2.183345 | -5.431105 | 0.434107  |
| 1  | -3.238211 | -4.843307 | -0.661568 |
| 7  | 6.583439  | 1.073937  | 0.021593  |
| 1  | 7.366781  | 0.493886  | -0.264821 |
| 1  | 6.752440  | 1.339420  | 0.987372  |
| 1  | 6.631874  | 1.925430  | -0.530119 |

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Cartesian coordinates of : BC9\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 5.923031  | 0.363143  | 0.164744  |
| 1  | 5.891576  | 1.174686  | -0.445484 |
| 1  | 4.209353  | -0.872529 | 0.155980  |
| 1  | 6.722692  | -0.191059 | -0.128749 |
| 1  | 6.133389  | 0.705881  | 1.097825  |
| 7  | 1.978600  | 1.504045  | -0.310424 |
| 1  | 2.357366  | 2.115030  | 0.408408  |
| 1  | -0.165593 | 1.537858  | -0.800341 |
| 1  | 2.318175  | 1.866798  | -1.197349 |
| 7  | 3.358403  | -1.446966 | 0.149513  |
| 1  | 3.293377  | -1.863191 | -0.776021 |
| 1  | 3.530392  | -2.218121 | 0.790412  |
| 1  | 2.408074  | 0.587176  | -0.177510 |
| 7  | 0.586421  | -0.663417 | 1.580400  |
| 1  | 1.439745  | -0.981166 | 1.111457  |
| 1  | 0.664006  | -0.918485 | 2.560898  |
| 1  | 0.607860  | 0.353206  | 1.527405  |
| 7  | -1.138007 | 1.437199  | -1.108631 |
| 1  | -1.128248 | 1.468559  | -2.124887 |
| 1  | -1.656497 | 2.265309  | -0.797348 |
| 1  | -1.695427 | -0.089291 | -0.456113 |
| 7  | -1.966978 | -3.301436 | -1.888709 |
| 1  | -2.712075 | -3.954426 | -1.661065 |
| 1  | -1.107076 | -3.842748 | -1.915995 |
| 1  | -2.140639 | -2.984057 | -2.838700 |
| 7  | -4.323279 | -1.015498 | 1.713139  |
| 1  | -4.365208 | -0.203473 | 2.323162  |
| 1  | -5.167760 | -0.996751 | 1.147630  |
| 1  | -4.393917 | -1.832653 | 2.313662  |
| 7  | -1.823362 | -1.017993 | 0.055000  |
| 1  | -1.856614 | -1.806338 | -0.617891 |
| 1  | -2.689369 | -1.009051 | 0.625962  |
| 1  | -0.980587 | -1.092520 | 0.674569  |
| 7  | -2.716475 | 4.075608  | -0.345111 |
| 1  | -2.257644 | 4.828436  | -0.850298 |
| 1  | -2.723453 | 4.344427  | 0.634444  |
| 1  | -3.684374 | 4.065701  | -0.653509 |

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Cartesian coordinates of : BDC9\_8

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.146399  | -0.587074 | 0.055087  |
| 1  | 1.571126  | 0.220709  | -0.305908 |
| 1  | 2.549590  | -0.371031 | 0.986704  |
| 1  | 1.461909  | -1.388557 | 0.128087  |
| 1  | 2.906069  | -0.821064 | -0.612995 |
| 7  | -4.373416 | -2.899834 | 0.542137  |
| 1  | -5.300999 | -2.667411 | 0.198691  |
| 1  | -4.182795 | -3.852745 | 0.246577  |
| 1  | -4.431885 | -2.911822 | 1.556079  |
| 7  | 0.211196  | 1.229805  | -0.967707 |
| 1  | -0.612830 | 0.645271  | -0.807508 |
| 1  | 0.012463  | 2.144714  | -0.559632 |
| 1  | 0.271105  | 1.371731  | -1.973015 |
| 7  | -2.884628 | 2.312306  | 0.103102  |
| 1  | -3.284142 | 2.402945  | 1.032579  |
| 1  | -2.041535 | 2.883620  | 0.074422  |
| 1  | -3.551942 | 2.722115  | -0.544080 |
| 7  | -0.263881 | 4.350302  | -0.018822 |
| 1  | -0.548661 | 4.754921  | 0.869604  |
| 1  | -0.683902 | 4.925859  | -0.744520 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.740355  | 4.495313  | -0.086818 |
| 7 | -2.431701 | -0.710013 | -0.737004 |
| 1 | -2.654444 | -0.738285 | -1.729230 |
| 1 | -3.053224 | -1.389602 | -0.287350 |
| 1 | -2.702177 | 0.220762  | -0.405576 |
| 7 | 0.002216  | -2.454418 | 0.101851  |
| 1 | -0.776726 | -1.850950 | -0.197056 |
| 1 | 0.047073  | -3.231666 | -0.551859 |
| 1 | -0.259810 | -2.851302 | 1.000351  |
| 7 | 3.315870  | -0.035695 | 2.756016  |
| 1 | 3.682946  | -0.885796 | 3.175799  |
| 1 | 4.080666  | 0.633823  | 2.743114  |
| 1 | 2.621848  | 0.329504  | 3.402834  |
| 7 | 4.325340  | -1.293793 | -1.870143 |
| 1 | 4.993929  | -0.541759 | -2.014768 |
| 1 | 3.953843  | -1.529817 | -2.786595 |
| 1 | 4.860388  | -2.100585 | -1.559546 |

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Cartesian coordinates of : BDC9\_9

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.509958 | 0.189806  | 0.145211  |
| 1  | -1.781334 | 0.500094  | 1.097891  |
| 1  | -2.374117 | -0.016767 | -0.420889 |
| 1  | -0.900502 | 0.918188  | -0.329323 |
| 1  | -0.923290 | -0.660943 | 0.195792  |
| 7  | 0.408590  | 1.820008  | -1.121740 |
| 1  | 0.539908  | 2.795097  | -0.831081 |
| 1  | 1.261775  | 1.304383  | -0.899882 |
| 1  | 0.320534  | 1.826844  | -2.134605 |
| 7  | -2.376168 | 1.103359  | 2.859769  |
| 1  | -2.965153 | 1.927895  | 2.777134  |
| 1  | -2.926296 | 0.403543  | 3.350704  |
| 1  | -1.609469 | 1.355529  | 3.477602  |
| 7  | -2.398974 | -3.297646 | -0.432773 |
| 1  | -2.808424 | -3.779106 | 0.362474  |
| 1  | -2.273556 | -3.994101 | -1.161834 |
| 1  | -1.473632 | -2.978225 | -0.154387 |
| 7  | 0.778079  | 4.874161  | -0.445812 |
| 1  | 1.466271  | 5.261570  | -1.085288 |
| 1  | -0.091763 | 5.369295  | -0.620924 |
| 1  | 1.075541  | 5.129816  | 0.491279  |
| 7  | -3.801352 | -0.681930 | -1.324255 |
| 1  | -3.584465 | -1.670112 | -1.161608 |
| 1  | -4.734086 | -0.498857 | -0.966076 |
| 1  | -3.837261 | -0.527203 | -2.327623 |
| 7  | 0.696816  | -1.840307 | -0.058323 |
| 1  | 1.016288  | -2.444613 | 0.695157  |
| 1  | 0.791432  | -2.381085 | -0.915224 |
| 1  | 1.390657  | -1.087299 | -0.130016 |
| 7  | 3.156139  | 0.190485  | -0.299267 |
| 1  | 3.381113  | 0.934278  | 0.357348  |
| 1  | 3.565576  | 0.466721  | -1.188861 |
| 1  | 3.681381  | -0.635561 | 0.010867  |
| 7  | 4.837519  | -2.319047 | 0.597235  |
| 1  | 4.747181  | -3.130808 | -0.007084 |
| 1  | 4.706179  | -2.646825 | 1.549926  |
| 1  | 5.804685  | -2.013971 | 0.528216  |

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Cartesian coordinates of : BL9\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X        | Y         | Z         |
|----|----------|-----------|-----------|
| 7  | 0.000033 | 0.526385  | 0.004190  |
| 1  | 0.864331 | -0.083735 | -0.000859 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.000873  | 1.120296  | 0.855392  |
| 1 | -0.000868 | 1.131780  | -0.838898 |
| 1 | -0.864200 | -0.083840 | 0.000901  |
| 7 | -0.002754 | 2.245338  | -2.452975 |
| 1 | 0.811764  | 2.850627  | -2.511026 |
| 1 | -0.002666 | 1.677729  | -3.296295 |
| 1 | -0.818555 | 2.848987  | -2.510090 |
| 7 | 2.328335  | -1.140837 | -0.009999 |
| 1 | 2.361167  | -1.748528 | -0.824913 |
| 1 | 3.205712  | -0.598593 | -0.010707 |
| 1 | 2.366766  | -1.755438 | 0.799465  |
| 7 | -2.328100 | -1.141105 | -0.005221 |
| 1 | -3.205519 | -0.598929 | -0.005781 |
| 1 | -2.365616 | -1.754538 | 0.805171  |
| 1 | -2.361752 | -1.749976 | -0.819220 |
| 7 | -7.345017 | -1.729072 | -0.002093 |
| 1 | -7.346434 | -2.328593 | 0.817876  |
| 1 | -7.339160 | -2.340444 | -0.813238 |
| 1 | -8.235361 | -1.239845 | -0.009583 |
| 7 | -4.994008 | 0.381956  | -0.007214 |
| 1 | -5.148510 | 0.969728  | -0.821717 |
| 1 | -5.739839 | -0.321795 | -0.005246 |
| 1 | -5.148046 | 0.973876  | 0.804363  |
| 7 | 0.002688  | 2.212125  | 2.484407  |
| 1 | 0.818551  | 2.814867  | 2.549662  |
| 1 | -0.811731 | 2.816730  | 2.550430  |
| 1 | 0.002419  | 1.633408  | 3.320148  |
| 7 | 4.994216  | 0.382270  | -0.012782 |
| 1 | 5.739968  | -0.321551 | -0.007728 |
| 1 | 5.149557  | 0.967257  | -0.829131 |
| 1 | 5.147534  | 0.976927  | 0.796925  |
| 7 | 7.344634  | -1.729369 | 0.001179  |
| 1 | 7.351601  | -2.318578 | 0.828565  |
| 1 | 8.235157  | -1.240815 | -0.018739 |
| 1 | 7.332667  | -2.350848 | -0.802177 |

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Cartesian coordinates of : Ca9

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.607510 | 1.930264  | -1.308286 |
| 1  | -0.005807 | 2.823472  | -0.383259 |
| 1  | -1.621241 | 2.176312  | -2.294988 |
| 1  | -1.672107 | 0.912108  | -1.257381 |
| 1  | -2.464349 | 2.304663  | -0.909745 |
| 7  | 1.061567  | -0.064236 | -1.653351 |
| 1  | 1.262649  | -0.052429 | -2.650989 |
| 1  | 1.026387  | 0.911298  | -1.361640 |
| 1  | 0.102095  | -0.410295 | -1.554803 |
| 7  | 1.662914  | 0.833831  | 1.597846  |
| 1  | 2.457715  | 0.328087  | 1.119988  |
| 1  | 1.943891  | 1.089808  | 2.542474  |
| 1  | 0.804278  | 0.200762  | 1.638956  |
| 7  | 0.853469  | 3.111525  | 0.105888  |
| 1  | 1.418512  | 1.710566  | 1.052677  |
| 1  | 1.489595  | 3.498579  | -0.586977 |
| 1  | 0.606509  | 3.884043  | 0.720010  |
| 7  | -1.859175 | -1.324380 | -1.221050 |
| 1  | -1.351703 | -2.143371 | -0.886371 |
| 1  | -2.345266 | -1.597569 | -2.071039 |
| 1  | -2.569759 | -1.104556 | -0.521607 |
| 7  | 0.772736  | -2.958345 | -0.263543 |
| 1  | 1.392831  | -3.345974 | 0.442525  |
| 1  | 1.253202  | -2.178625 | -0.712887 |
| 1  | 0.651780  | -3.687133 | -0.962132 |
| 7  | 3.655815  | -0.504465 | 0.069485  |
| 1  | 3.044600  | -0.592221 | -0.745064 |
| 1  | 3.996509  | -1.429018 | 0.317215  |
| 1  | 4.468830  | 0.040796  | -0.203949 |

|   |           |           |          |
|---|-----------|-----------|----------|
| 7 | -0.581523 | -0.868796 | 1.646217 |
| 1 | -1.441140 | -0.459835 | 1.277328 |
| 1 | -0.809981 | -1.249897 | 2.561236 |
| 1 | -0.342304 | -1.661062 | 1.042507 |
| 7 | -3.798158 | -0.127972 | 1.103346 |
| 1 | -4.544025 | 0.116011  | 0.455707 |
| 1 | -3.732506 | 0.647026  | 1.758813 |
| 1 | -4.140146 | -0.923529 | 1.637524 |

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Cartesian coordinates of : BL9\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.000000  | -0.783292 | 0.000020  |
| 1  | 0.858910  | -0.171713 | 0.140735  |
| 1  | 0.137815  | -1.382315 | -0.833243 |
| 1  | -0.137814 | -1.382269 | 0.833315  |
| 1  | -0.858912 | -0.171724 | -0.140729 |
| 7  | -0.426813 | -2.488405 | 2.457523  |
| 1  | -0.426268 | -3.489426 | 2.282391  |
| 1  | 0.287763  | -2.314968 | 3.159078  |
| 1  | -1.320062 | -2.268705 | 2.889770  |
| 7  | 2.281303  | 0.863537  | 0.380404  |
| 1  | 2.097858  | 1.573602  | 1.085134  |
| 1  | 3.109649  | 0.349891  | 0.697365  |
| 1  | 2.542260  | 1.367960  | -0.472866 |
| 7  | -2.281312 | 0.863510  | -0.380456 |
| 1  | -3.109665 | 0.349840  | -0.697359 |
| 1  | -2.097874 | 1.573514  | -1.085249 |
| 1  | -2.542255 | 1.368008  | 0.472775  |
| 7  | -3.150903 | 2.584628  | 2.161002  |
| 1  | -3.576367 | 3.428658  | 1.788226  |
| 1  | -2.406728 | 2.883353  | 2.784379  |
| 1  | -3.854656 | 2.134414  | 2.738851  |
| 7  | -4.933055 | -0.569975 | -1.423475 |
| 1  | -5.075467 | -1.547473 | -1.187272 |
| 1  | -5.707995 | -0.054557 | -1.015920 |
| 1  | -5.031783 | -0.494344 | -2.431721 |
| 7  | 0.426813  | -2.488541 | -2.457389 |
| 1  | 1.320083  | -2.268907 | -2.889626 |
| 1  | 0.426214  | -3.489554 | -2.282210 |
| 1  | -0.287737 | -2.315103 | -3.158971 |
| 7  | 4.933026  | -0.569866 | 1.423572  |
| 1  | 5.707964  | -0.054412 | 1.016058  |
| 1  | 5.031715  | -0.494257 | 2.431823  |
| 1  | 5.075479  | -1.547352 | 1.187350  |
| 7  | 3.150942  | 2.584422  | -2.161198 |
| 1  | 2.406755  | 2.883188  | -2.784542 |
| 1  | 3.854612  | 2.134106  | -2.739069 |
| 1  | 3.576513  | 3.428430  | -1.788495 |

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Cartesian coordinates of : BTC9\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.658594 | 0.004856  | 0.162523  |
| 1  | -0.207306 | -0.890639 | -0.139647 |
| 1  | -0.595826 | 0.083022  | 1.201829  |
| 1  | -0.171590 | 0.819245  | -0.266150 |
| 1  | -1.660626 | 0.006405  | -0.112607 |
| 7  | 2.681696  | -0.336326 | -0.957653 |
| 1  | 3.579402  | -0.267413 | -0.467032 |
| 1  | 2.897947  | -0.588772 | -1.918759 |
| 1  | 2.167758  | -1.121349 | -0.564433 |
| 7  | -3.540957 | 0.395481  | -0.516727 |
| 1  | -4.321384 | 0.277540  | 0.124871  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -3.915799 | 0.253157  | -1.451709 |
| 1 | -3.252638 | 1.381015  | -0.459785 |
| 7 | -2.104713 | 3.107755  | -0.339405 |
| 1 | -2.421218 | 3.720358  | -1.086292 |
| 1 | -2.201207 | 3.635351  | 0.523524  |
| 1 | -1.109968 | 2.941410  | -0.487599 |
| 7 | 0.262377  | -2.661630 | -0.562569 |
| 1 | 0.567778  | -2.880950 | -1.507510 |
| 1 | 0.801156  | -3.257468 | 0.060817  |
| 1 | -0.721543 | -2.950756 | -0.488818 |
| 7 | 1.008517  | 2.185931  | -0.963248 |
| 1 | 1.711420  | 1.430289  | -0.993229 |
| 1 | 1.410923  | 2.943317  | -0.416333 |
| 1 | 0.916619  | 2.537711  | -1.913467 |
| 7 | -2.787601 | -2.839018 | -0.309714 |
| 1 | -3.209824 | -3.322828 | -1.097451 |
| 1 | -3.164572 | -3.270509 | 0.529263  |
| 1 | -3.117388 | -1.875219 | -0.333811 |
| 7 | 5.559383  | -0.089099 | 0.319727  |
| 1 | 5.641826  | 0.090007  | 1.316180  |
| 1 | 6.093129  | -0.932580 | 0.129920  |
| 1 | 6.038710  | 0.671577  | -0.153679 |
| 7 | -0.477766 | 0.211929  | 3.098847  |
| 1 | -0.372856 | -0.699315 | 3.537708  |
| 1 | -1.299725 | 0.640297  | 3.516891  |
| 1 | 0.320411  | 0.767951  | 3.394834  |

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Cartesian coordinates of : BCa9

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.062607 | 0.845886  | 1.931780  |
| 1  | -1.236890 | -1.130738 | 2.212613  |
| 1  | -1.542649 | 1.234332  | 2.715863  |
| 1  | -1.958420 | 1.513835  | 1.160671  |
| 1  | -3.040591 | 0.865052  | 2.211912  |
| 7  | 0.808355  | 0.553708  | 0.254400  |
| 1  | 1.584460  | 1.033940  | 0.724207  |
| 1  | 0.428793  | -0.116172 | 0.921656  |
| 1  | 0.066277  | 1.242123  | 0.120400  |
| 7  | -0.097878 | -2.662831 | -0.410341 |
| 1  | 0.863849  | -2.389419 | -0.758545 |
| 1  | -0.311155 | -3.620661 | -0.680482 |
| 1  | -0.837042 | -1.988236 | -0.787454 |
| 7  | -0.685753 | -1.990968 | 2.312034  |
| 1  | -0.163443 | -2.555225 | 0.633833  |
| 1  | 0.044896  | -1.806299 | 2.994991  |
| 1  | -1.293860 | -2.689454 | 2.733024  |
| 7  | -1.712609 | 2.598696  | -0.693855 |
| 1  | -1.336043 | 2.201073  | -1.557049 |
| 1  | -1.275179 | 3.508240  | -0.567454 |
| 1  | -2.697707 | 2.786598  | -0.865541 |
| 7  | -0.015990 | 0.880329  | -2.790917 |
| 1  | -0.063399 | 0.123385  | -3.467500 |
| 1  | 0.564588  | 0.578602  | -2.006800 |
| 1  | 0.459941  | 1.649365  | -3.254981 |
| 7  | 2.419448  | -1.675376 | -1.250584 |
| 1  | 2.228785  | -0.734065 | -0.900326 |
| 1  | 2.638161  | -1.609860 | -2.240734 |
| 1  | 3.254440  | -2.023906 | -0.788027 |
| 7  | -2.020061 | -0.738525 | -1.004405 |
| 1  | -2.126773 | -0.299443 | -0.088381 |
| 1  | -2.945840 | -1.011335 | -1.323265 |
| 1  | -1.670846 | -0.019026 | -1.639860 |
| 7  | 3.303139  | 1.999861  | 1.562983  |
| 1  | 3.938169  | 2.318217  | 0.836227  |
| 1  | 3.855747  | 1.436285  | 2.202987  |
| 1  | 3.019419  | 2.827335  | 2.080358  |

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Cartesian coordinates of : TC9\_3

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 3.291754  | -2.573498 | 0.378168  |
| 1  | 1.772041  | -2.006429 | -0.333868 |
| 1  | 3.921662  | -3.088625 | -0.230632 |
| 1  | 3.736947  | -1.676239 | 0.607132  |
| 1  | 3.214264  | -3.111202 | 1.236992  |
| 7  | 0.936781  | -1.489622 | -0.735864 |
| 1  | 1.029942  | -1.451205 | -1.748877 |
| 1  | 0.028547  | -1.970027 | -0.495671 |
| 1  | 0.931593  | -0.485879 | -0.346302 |
| 7  | -4.194098 | -1.054518 | -0.233590 |
| 1  | -4.611440 | -0.940728 | -1.153928 |
| 1  | -4.236930 | -0.142154 | 0.223022  |
| 1  | -4.812021 | -1.676303 | 0.281828  |
| 7  | -2.043902 | 1.238040  | -0.931434 |
| 1  | -2.219538 | 0.262013  | -1.158865 |
| 1  | -2.784866 | 1.507014  | -0.283540 |
| 1  | -2.180139 | 1.774431  | -1.783592 |
| 7  | -1.558794 | -2.761287 | -0.086635 |
| 1  | -1.531167 | -3.109880 | 0.868569  |
| 1  | -1.749828 | -3.568392 | -0.675523 |
| 1  | -2.379594 | -2.147059 | -0.151782 |
| 7  | 0.809747  | 1.107199  | 0.241704  |
| 1  | 1.516485  | 1.761980  | -0.098523 |
| 1  | -0.115150 | 1.389480  | -0.104272 |
| 1  | 0.793336  | 1.181064  | 1.255245  |
| 7  | 3.194731  | 3.085524  | -0.714831 |
| 1  | 2.557617  | 3.784955  | -1.088507 |
| 1  | 3.740932  | 3.556406  | 0.002315  |
| 1  | 3.839627  | 2.861050  | -1.468395 |
| 7  | 4.232184  | 0.334475  | 0.899717  |
| 1  | 3.685351  | 1.010403  | 0.367903  |
| 1  | 5.208765  | 0.482379  | 0.660138  |
| 1  | 4.135604  | 0.578760  | 1.881459  |
| 7  | -4.551066 | 1.929329  | 1.137908  |
| 1  | -5.420642 | 2.172418  | 0.669952  |
| 1  | -4.082989 | 2.808660  | 1.343395  |
| 1  | -4.809770 | 1.533613  | 2.038324  |

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Cartesian coordinates of : BC9\_3

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -4.970528 | 0.070404  | 0.862471  |
| 1  | -3.200009 | 0.295918  | -0.062683 |
| 1  | -5.031124 | 0.536506  | 1.763724  |
| 1  | -5.701317 | 0.479634  | 0.270280  |
| 1  | -5.235509 | -0.897382 | 1.024749  |
| 7  | -7.292876 | 1.297965  | -0.884055 |
| 1  | -7.218221 | 2.302620  | -1.014150 |
| 1  | -7.375413 | 0.887268  | -1.809425 |
| 1  | -8.174616 | 1.128727  | -0.408513 |
| 7  | -2.284940 | 0.403146  | -0.531040 |
| 1  | -2.118009 | 1.401482  | -0.629344 |
| 1  | -1.055245 | -0.429316 | 0.379122  |
| 1  | -2.391952 | 0.039196  | -1.474715 |
| 7  | 0.532642  | -3.337805 | -0.254837 |
| 1  | 1.533152  | -3.140766 | -0.395707 |
| 1  | 0.462085  | -4.188699 | 0.296966  |
| 1  | 0.130125  | -3.549962 | -1.163823 |
| 7  | -0.346292 | -0.966026 | 0.973056  |
| 1  | -0.081855 | -1.886616 | 0.504233  |
| 1  | -0.769074 | -1.165082 | 1.877769  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 0.531158 | -0.400259 | 1.124190  |
| 7 | 3.472868 | -2.487999 | -0.566911 |
| 1 | 3.578837 | -1.473277 | -0.578723 |
| 1 | 4.066548 | -2.844442 | 0.176836  |
| 1 | 3.861338 | -2.839845 | -1.437739 |
| 7 | 4.197513 | 0.691906  | -0.938687 |
| 1 | 5.150593 | 0.335525  | -0.935779 |
| 1 | 3.901051 | 0.698354  | -1.911736 |
| 1 | 4.262226 | 1.674292  | -0.647326 |
| 7 | 2.100260 | 0.481596  | 1.421168  |
| 1 | 1.974570 | 1.471088  | 1.620049  |
| 1 | 2.599473 | 0.094075  | 2.218244  |
| 1 | 2.739451 | 0.427765  | 0.620892  |
| 7 | 4.540651 | 3.688391  | -0.022404 |
| 1 | 5.263022 | 4.045912  | -0.641832 |
| 1 | 4.900167 | 3.780363  | 0.923515  |
| 1 | 3.753465 | 4.325875  | -0.100402 |

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Cartesian coordinates of : BL9\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.569953 | 0.309212  | -0.738869 |
| 1  | -1.333048 | -0.285833 | -0.258804 |
| 1  | -0.396732 | -0.072135 | -1.666944 |
| 1  | -0.892733 | 1.307892  | -0.843159 |
| 1  | 0.338554  | 0.272820  | -0.188701 |
| 7  | -1.443131 | 3.032029  | -1.082235 |
| 1  | -2.296557 | 3.086723  | -1.632726 |
| 1  | -1.633622 | 3.516752  | -0.196521 |
| 1  | -0.751975 | 3.590625  | -1.576888 |
| 7  | -2.545324 | -1.233912 | 0.460436  |
| 1  | -3.006045 | -0.738977 | 1.220303  |
| 1  | -3.279998 | -1.488670 | -0.209289 |
| 1  | -2.179191 | -2.105039 | 0.860369  |
| 7  | 1.893661  | 0.195675  | 0.662829  |
| 1  | 2.657394  | -0.042100 | 0.010365  |
| 1  | 1.903338  | -0.505400 | 1.399287  |
| 1  | 2.146909  | 1.075645  | 1.105098  |
| 7  | 6.947239  | -0.460244 | 0.194220  |
| 1  | 7.016612  | -1.132086 | 0.952886  |
| 1  | 7.190375  | 0.446694  | 0.581654  |
| 1  | 7.673601  | -0.697474 | -0.475316 |
| 7  | 4.153416  | -0.493314 | -1.279848 |
| 1  | 4.241956  | 0.164987  | -2.049159 |
| 1  | 5.044880  | -0.475904 | -0.773311 |
| 1  | 4.075254  | -1.414607 | -1.701837 |
| 7  | -2.071167 | 4.654517  | 1.516262  |
| 1  | -2.879076 | 4.319143  | 2.033047  |
| 1  | -1.306428 | 4.721574  | 2.181715  |
| 1  | -2.286625 | 5.603897  | 1.224469  |
| 7  | -4.857166 | -2.037758 | -1.547331 |
| 1  | -5.593185 | -2.473466 | -0.998709 |
| 1  | -5.287943 | -1.269169 | -2.052992 |
| 1  | -4.569632 | -2.720233 | -2.242831 |
| 7  | -1.539349 | -3.943827 | 1.751505  |
| 1  | -0.777158 | -4.419315 | 1.277391  |
| 1  | -2.332747 | -4.578503 | 1.737559  |
| 1  | -1.263747 | -3.844482 | 2.724262  |

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Cartesian coordinates of : BL9\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y        | Z        |
|----|-----------|----------|----------|
| 7  | -0.001585 | 0.572603 | 0.602705 |
| 1  | 0.876208  | 0.331559 | 0.045882 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.002333 | 0.017853  | 1.456748  |
| 1 | -0.001752 | 1.597092  | 0.867174  |
| 1 | -0.878652 | 0.331961  | 0.044617  |
| 7 | -0.004021 | 3.328324  | 1.377520  |
| 1 | 0.800720  | 3.557599  | 1.955831  |
| 1 | 0.009478  | 3.980664  | 0.583252  |
| 1 | -0.824648 | 3.561467  | 1.931460  |
| 7 | 2.341590  | -0.110422 | -0.809108 |
| 1 | 2.893763  | 0.695769  | -1.090984 |
| 1 | 2.947430  | -0.693600 | -0.209057 |
| 1 | 2.165373  | -0.643582 | -1.657051 |
| 7 | -2.343382 | -0.108562 | -0.812609 |
| 1 | -2.952579 | -0.687640 | -0.211982 |
| 1 | -2.166598 | -0.645454 | -1.658081 |
| 1 | -2.892448 | 0.698177  | -1.098964 |
| 7 | -6.703500 | -2.718696 | -0.647213 |
| 1 | -6.494834 | -3.348971 | -1.416003 |
| 1 | -7.237140 | -1.946986 | -1.036379 |
| 1 | -7.325893 | -3.218590 | -0.018793 |
| 7 | -4.142450 | -1.816143 | 0.960987  |
| 1 | -4.489413 | -1.331977 | 1.784567  |
| 1 | -4.964682 | -2.093988 | 0.414416  |
| 1 | -3.711534 | -2.673605 | 1.295775  |
| 7 | 0.035460  | 5.441138  | -0.919686 |
| 1 | 0.895623  | 5.457270  | -1.460221 |
| 1 | -0.726828 | 5.367783  | -1.587369 |
| 1 | -0.049007 | 6.354448  | -0.481824 |
| 7 | 4.130213  | -1.830273 | 0.963293  |
| 1 | 4.951213  | -2.112232 | 0.416978  |
| 1 | 4.479384  | -1.348773 | 1.787502  |
| 1 | 3.694341  | -2.685619 | 1.297076  |
| 7 | 6.687277  | -2.746281 | -0.643689 |
| 1 | 6.475888  | -3.378037 | -1.410516 |
| 1 | 7.308074  | -3.246657 | -0.014073 |
| 1 | 7.223634  | -1.977743 | -1.035383 |

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Cartesian coordinates of : BL9\_7

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.101636  | 0.917046  | 0.565937  |
| 1  | -0.252982 | 1.713833  | -0.034675 |
| 1  | 0.541498  | 1.307030  | 1.397326  |
| 1  | -0.709719 | 0.294073  | 0.867702  |
| 1  | 0.830349  | 0.345583  | 0.035027  |
| 7  | -2.043654 | -0.732070 | 1.374826  |
| 1  | -2.649215 | -0.290686 | 2.062706  |
| 1  | -2.642788 | -0.988272 | 0.573612  |
| 1  | -1.729421 | -1.603607 | 1.794815  |
| 7  | -0.860356 | 3.075554  | -1.037676 |
| 1  | -1.843838 | 2.953195  | -1.266035 |
| 1  | -0.774070 | 3.990202  | -0.576245 |
| 1  | -0.369873 | 3.147517  | -1.925665 |
| 7  | 2.065349  | -0.590563 | -0.781529 |
| 1  | 2.904065  | -0.685928 | -0.186046 |
| 1  | 2.372175  | -0.175767 | -1.657958 |
| 1  | 1.754969  | -1.532365 | -1.007530 |
| 7  | -3.858104 | -1.536946 | -0.945926 |
| 1  | -4.554358 | -2.193739 | -0.577421 |
| 1  | -3.381196 | -2.011506 | -1.707657 |
| 1  | -4.374804 | -0.770200 | -1.367811 |
| 7  | 4.544906  | -0.868330 | 0.971377  |
| 1  | 4.993734  | 0.014590  | 1.199508  |
| 1  | 4.380431  | -1.340831 | 1.856087  |
| 1  | 5.237674  | -1.428011 | 0.462626  |
| 7  | 6.734820  | -2.579512 | -0.523810 |
| 1  | 6.425745  | -3.516032 | -0.767089 |
| 1  | 7.069831  | -2.148850 | -1.380610 |
| 1  | 7.540777  | -2.685639 | 0.085573  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -0.639321 | 5.895341  | 0.273869  |
| 1 | -1.002749 | 6.571691  | -0.392064 |
| 1 | -1.181617 | 6.007499  | 1.125809  |
| 1 | 0.309692  | 6.185324  | 0.492292  |
| 7 | -6.039502 | -3.549771 | 0.127367  |
| 1 | -6.651475 | -3.821678 | -0.636650 |
| 1 | -6.631271 | -3.146188 | 0.847640  |
| 1 | -5.651986 | -4.406482 | 0.511684  |

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Cartesian coordinates of : BDC9\_10

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.608744  | -1.417542 | -0.708828 |
| 1  | 1.398671  | -0.568496 | -0.076577 |
| 1  | 1.487485  | -1.138638 | -1.680538 |
| 1  | 2.587183  | -1.751098 | -0.576592 |
| 1  | 0.917625  | -2.210530 | -0.488513 |
| 7  | 0.965283  | 0.753213  | 0.905609  |
| 1  | 1.407562  | 1.642296  | 0.662646  |
| 1  | -0.051224 | 0.891921  | 0.826542  |
| 1  | 1.163989  | 0.589833  | 1.889835  |
| 7  | -2.034605 | 1.371238  | 0.450322  |
| 1  | -1.650020 | 2.081891  | -0.178984 |
| 1  | -2.710634 | 0.809513  | -0.065832 |
| 1  | -2.553465 | 1.860599  | 1.174603  |
| 7  | -2.357018 | -1.664120 | 1.210950  |
| 1  | -2.799887 | -2.060632 | 2.034884  |
| 1  | -1.916583 | -0.788799 | 1.487604  |
| 1  | -3.099794 | -1.392157 | 0.565291  |
| 7  | -4.629092 | -0.388341 | -0.811413 |
| 1  | -4.556372 | 0.136863  | -1.678895 |
| 1  | -5.314747 | 0.095697  | -0.237486 |
| 1  | -5.042412 | -1.284314 | -1.057253 |
| 7  | -0.278862 | 3.451005  | -1.109902 |
| 1  | 0.636195  | 3.397694  | -0.664666 |
| 1  | -0.139883 | 3.351220  | -2.110932 |
| 1  | -0.636342 | 4.389828  | -0.957833 |
| 7  | 2.583652  | 3.607961  | 0.541101  |
| 1  | 3.410877  | 3.167549  | 0.935989  |
| 1  | 2.917882  | 4.212765  | -0.205297 |
| 1  | 2.215167  | 4.221050  | 1.264297  |
| 7  | -0.253888 | -3.399985 | -0.092187 |
| 1  | 0.062115  | -4.106795 | 0.567034  |
| 1  | -1.024408 | -2.879916 | 0.360045  |
| 1  | -0.648535 | -3.902886 | -0.882932 |
| 7  | 4.364785  | -2.451039 | -0.373710 |
| 1  | 4.623266  | -2.552861 | 0.604410  |
| 1  | 5.083153  | -1.873868 | -0.803347 |
| 1  | 4.450157  | -3.374464 | -0.791096 |

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Cartesian coordinates of : BTC9\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.084044 | 0.666347  | -0.600885 |
| 1  | 0.709403  | 1.341172  | -0.393063 |
| 1  | -0.127800 | 0.498804  | -1.604954 |
| 1  | 0.075759  | -0.265876 | -0.118228 |
| 1  | -0.999494 | 1.076622  | -0.313532 |
| 7  | 3.332458  | -0.436147 | 0.569721  |
| 1  | 4.079645  | -1.047840 | 0.221709  |
| 1  | 3.639552  | -0.089706 | 1.474921  |
| 1  | 3.286868  | 0.369324  | -0.048972 |
| 7  | -2.848800 | 1.476177  | -0.037203 |
| 1  | -3.433366 | 2.016739  | -0.670162 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -3.236876 | 1.602818  | 0.894262  |
| 1 | -2.972183 | 0.484294  | -0.284798 |
| 7 | -2.535939 | -1.479702 | -0.736278 |
| 1 | -3.364321 | -1.947924 | -0.350113 |
| 1 | -2.470153 | -1.774940 | -1.707023 |
| 1 | -1.723320 | -1.862181 | -0.257778 |
| 7 | 1.822583  | 2.681065  | -0.043039 |
| 1 | 2.341375  | 2.651599  | 0.830807  |
| 1 | 2.463572  | 3.022125  | -0.754647 |
| 1 | 1.076595  | 3.380937  | 0.067259  |
| 7 | 0.631246  | -1.773266 | 0.645662  |
| 1 | 1.611080  | -1.453518 | 0.717844  |
| 1 | 0.644258  | -2.661199 | 0.149853  |
| 1 | 0.302674  | -1.970717 | 1.587588  |
| 7 | -0.835793 | 4.146111  | 0.221173  |
| 1 | -0.965200 | 4.630012  | 1.105291  |
| 1 | -1.056247 | 4.815818  | -0.510495 |
| 1 | -1.532001 | 3.403701  | 0.175559  |
| 7 | 5.668102  | -2.311867 | -0.375138 |
| 1 | 5.574158  | -2.706484 | -1.306510 |
| 1 | 6.552128  | -1.811229 | -0.358500 |
| 1 | 5.764665  | -3.094899 | 0.265117  |
| 7 | -5.131811 | -2.886008 | 0.336334  |
| 1 | -5.104186 | -3.884404 | 0.149345  |
| 1 | -5.944357 | -2.521133 | -0.152684 |
| 1 | -5.318234 | -2.780897 | 1.329469  |

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Cartesian coordinates of : L9

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Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | -0.000002  | -0.721786 | -0.000739 |
| 1  | 0.896880   | -0.101989 | 0.179002  |
| 1  | -0.165898  | -1.322129 | 0.805710  |
| 1  | -0.896926  | -0.101941 | -0.180105 |
| 1  | 0.165934   | -1.321632 | -0.807549 |
| 7  | -2.238396  | 0.763307  | -0.415105 |
| 1  | -2.392596  | 1.021509  | -1.387342 |
| 1  | -3.068383  | 0.213486  | -0.114161 |
| 1  | -2.251279  | 1.632561  | 0.113916  |
| 7  | 2.238297   | 0.763194  | 0.414539  |
| 1  | 2.392216   | 1.021241  | 1.386861  |
| 1  | 3.068358   | 0.213398  | 0.113755  |
| 1  | 2.251361   | 1.632530  | -0.114343 |
| 7  | 7.022456   | 0.837330  | 0.628725  |
| 1  | 7.028255   | 1.801153  | 0.306827  |
| 1  | 7.071504   | 0.874494  | 1.643040  |
| 1  | 7.896156   | 0.410621  | 0.304914  |
| 7  | 4.629678   | -0.794226 | -0.430162 |
| 1  | 5.432352   | -0.252670 | -0.077843 |
| 1  | 4.758233   | -0.885651 | -1.434483 |
| 1  | 4.719981   | -1.731490 | -0.047047 |
| 7  | -7.022589  | 0.837295  | -0.628381 |
| 1  | -7.896210  | 0.410591  | -0.304349 |
| 1  | -7.028336  | 1.801140  | -0.306551 |
| 1  | -7.071857  | 0.874384  | -1.642688 |
| 7  | -4.629565  | -0.794189 | 0.430066  |
| 1  | -4.719932  | -1.731462 | 0.046991  |
| 1  | -4.757912  | -0.885593 | 1.434416  |
| 1  | -5.432319  | -0.252652 | 0.077900  |
| 7  | 9.758727   | -0.434862 | -0.331095 |
| 1  | 9.923087   | -1.354663 | 0.067043  |
| 1  | 10.533760  | 0.154585  | -0.041805 |
| 1  | 9.823751   | -0.533808 | -1.339795 |
| 7  | -9.758609  | -0.434914 | 0.332124  |
| 1  | -10.533749 | 0.154307  | 0.042656  |
| 1  | -9.823548  | -0.533470 | 1.340867  |
| 1  | -9.922863  | -1.354895 | -0.065639 |

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Cartesian coordinates of the protonated ammonia decamer

Cartesian coordinates of : BCa10\_1

| -----                                        |           |           |           |
|----------------------------------------------|-----------|-----------|-----------|
| Atomic number (AN) and Cartesian coordinates |           |           |           |
| AN                                           | X         | Y         | Z         |
| -----                                        |           |           |           |
| 7                                            | 1.137887  | 0.261279  | -1.665322 |
| 1                                            | 1.075406  | 0.499757  | -2.651277 |
| 1                                            | 1.547566  | 1.063250  | -1.184195 |
| 1                                            | -0.460987 | -0.120820 | -0.805110 |
| 1                                            | 1.801186  | -0.509224 | -1.578715 |
| 7                                            | -1.263080 | -0.139595 | -0.128500 |
| 1                                            | -2.190704 | -0.127969 | -0.631712 |
| 1                                            | -1.178634 | -0.982283 | 0.482800  |
| 1                                            | -1.135611 | 0.718732  | 0.438274  |
| 7                                            | -0.280287 | 2.419425  | 1.034331  |
| 1                                            | -0.875431 | 3.139706  | 0.631950  |
| 1                                            | -0.215294 | 2.633645  | 2.026420  |
| 1                                            | 0.655399  | 2.549873  | 0.635242  |
| 7                                            | 4.338100  | -0.136422 | -0.550210 |
| 1                                            | 4.772231  | 0.218185  | -1.399316 |
| 1                                            | 5.104888  | -0.380594 | 0.072004  |
| 1                                            | 3.867494  | -1.008374 | -0.804303 |
| 7                                            | -3.776294 | -0.127947 | -1.518296 |
| 1                                            | -4.582892 | 0.033333  | -0.901919 |
| 1                                            | -3.817908 | 0.582398  | -2.244966 |
| 1                                            | -3.940567 | -1.016942 | -1.984438 |
| 7                                            | 2.756433  | 2.568100  | 0.072268  |
| 1                                            | 3.374502  | 1.763209  | -0.068154 |
| 1                                            | 2.979841  | 3.246508  | -0.652153 |
| 1                                            | 3.037660  | 2.998398  | 0.950525  |
| 7                                            | 2.266802  | -2.534352 | -0.700470 |
| 1                                            | 1.530492  | -2.906867 | -1.293597 |
| 1                                            | 2.844977  | -3.323653 | -0.425265 |
| 1                                            | 1.836896  | -2.150582 | 0.141585  |
| 7                                            | -0.664797 | -2.373740 | 1.643215  |
| 1                                            | -0.567413 | -3.315723 | 1.275137  |
| 1                                            | -1.169748 | -2.454491 | 2.521241  |
| 1                                            | 0.269520  | -2.016431 | 1.848388  |
| 7                                            | 1.758365  | -0.321983 | 1.521711  |
| 1                                            | 2.060778  | -0.223027 | 2.488139  |
| 1                                            | 1.096597  | 0.433490  | 1.346407  |
| 1                                            | 2.574238  | -0.115822 | 0.941662  |
| 7                                            | -6.321211 | 0.332135  | 0.230273  |
| 1                                            | -7.124223 | 0.062325  | -0.331255 |
| 1                                            | -6.468973 | 1.300332  | 0.500701  |
| 1                                            | -6.364702 | -0.218639 | 1.082897  |
| -----                                        |           |           |           |

Cartesian coordinates of : BCa10\_2

| -----                                        |           |           |           |
|----------------------------------------------|-----------|-----------|-----------|
| Atomic number (AN) and Cartesian coordinates |           |           |           |
| AN                                           | X         | Y         | Z         |
| -----                                        |           |           |           |
| 7                                            | -1.627472 | -2.051777 | 1.857310  |
| 1                                            | 0.129103  | -0.927052 | 2.465422  |
| 1                                            | -2.223589 | -1.532213 | 2.497928  |
| 1                                            | -2.115149 | -2.062700 | 0.955270  |
| 1                                            | -1.615665 | -3.008780 | 2.202124  |
| 7                                            | -1.253264 | 0.746233  | 0.050780  |
| 1                                            | -1.862195 | 1.481941  | 0.425214  |
| 1                                            | -0.624682 | 0.466742  | 0.802402  |
| 1                                            | -1.840410 | -0.070088 | -0.125098 |
| 7                                            | 2.176035  | 0.231885  | 0.115479  |
| 1                                            | 1.869257  | 1.094501  | -0.393493 |
| 1                                            | 3.211119  | 0.134062  | 0.085512  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.696797  | -0.610939 | -0.299261 |
| 7 | 0.854672  | -0.240125 | 2.697454  |
| 1 | 1.833451  | 0.258287  | 1.098168  |
| 1 | 0.408231  | 0.496879  | 3.237554  |
| 1 | 1.506423  | -0.697507 | 3.330264  |
| 7 | -2.801539 | -2.024266 | -1.093575 |
| 1 | -2.242411 | -1.660341 | -1.868627 |
| 1 | -3.747129 | -1.669494 | -1.213531 |
| 1 | -2.863448 | -3.031091 | -1.225423 |
| 7 | -0.802032 | -0.311113 | -2.887470 |
| 1 | 0.112531  | -0.335947 | -3.329685 |
| 1 | -0.762655 | 0.334143  | -2.096296 |
| 1 | -1.446214 | 0.070837  | -3.574459 |
| 7 | 1.003145  | 2.512926  | -1.225136 |
| 1 | 0.056654  | 2.200226  | -0.997367 |
| 1 | 1.067809  | 2.616140  | -2.233760 |
| 1 | 1.135313  | 3.438144  | -0.826727 |
| 7 | 0.571867  | -2.003399 | -0.615767 |
| 1 | -0.018822 | -2.076613 | 0.214133  |
| 1 | 0.978514  | -2.919817 | -0.781497 |
| 1 | -0.045646 | -1.793452 | -1.400814 |
| 7 | -3.124762 | 3.115339  | 1.034050  |
| 1 | -3.267800 | 3.755866  | 0.258257  |
| 1 | -2.791777 | 3.674275  | 1.814432  |
| 1 | -4.043595 | 2.770234  | 1.297256  |
| 7 | 5.137427  | -0.014988 | 0.019913  |
| 1 | 5.489027  | 0.045423  | -0.932213 |
| 1 | 5.482483  | -0.892830 | 0.399376  |
| 1 | 5.595938  | 0.726144  | 0.543674  |

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Cartesian coordinates of : BTC10\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.168387 | -1.724693 | -0.077133 |
| 1  | -1.569998 | -1.568386 | 0.876734  |
| 1  | -1.507375 | -0.955509 | -0.706571 |
| 1  | -0.136227 | -1.575956 | 0.017682  |
| 1  | -1.404555 | -2.663759 | -0.447897 |
| 7  | 1.418759  | -0.608529 | 0.368913  |
| 1  | 1.214295  | -0.170357 | 1.265080  |
| 1  | 2.383628  | -0.939447 | 0.402460  |
| 1  | 1.389909  | 0.146330  | -0.316837 |
| 7  | -1.875931 | -0.780762 | 2.533708  |
| 1  | -1.398846 | -1.165656 | 3.343578  |
| 1  | -1.438187 | 0.115098  | 2.295573  |
| 1  | -2.833857 | -0.597071 | 2.816912  |
| 7  | -1.893342 | -4.436615 | -1.110215 |
| 1  | -1.360247 | -4.714950 | -1.929718 |
| 1  | -2.874442 | -4.487430 | -1.371576 |
| 1  | -1.743441 | -5.156397 | -0.408153 |
| 7  | 1.178715  | 2.106902  | -1.585072 |
| 1  | 1.380247  | 1.832363  | -2.544279 |
| 1  | 2.081168  | 2.097378  | -1.091874 |
| 1  | 0.879760  | 3.078504  | -1.632842 |
| 7  | 3.833631  | 1.688487  | -0.028869 |
| 1  | 4.643943  | 2.051294  | -0.523339 |
| 1  | 3.836608  | 2.122903  | 0.889783  |
| 1  | 3.982412  | 0.689381  | 0.112448  |
| 7  | -1.748586 | 0.629452  | -1.626981 |
| 1  | -2.369059 | 1.257745  | -1.114004 |
| 1  | -0.828480 | 1.074257  | -1.662834 |
| 1  | -2.095960 | 0.569417  | -2.579925 |
| 7  | 4.581489  | -1.533783 | 0.396755  |
| 1  | 5.036139  | -1.635289 | -0.507172 |
| 1  | 5.304320  | -1.250544 | 1.053697  |
| 1  | 4.296736  | -2.469070 | 0.677174  |
| 7  | -0.720885 | 1.791773  | 1.153318  |
| 1  | -0.394811 | 2.527680  | 1.774622  |

|   |           |          |           |
|---|-----------|----------|-----------|
| 1 | -1.632515 | 2.085066 | 0.798764  |
| 1 | -0.089530 | 1.783851 | 0.351348  |
| 7 | -3.704264 | 2.730445 | -0.006042 |
| 1 | -3.592320 | 3.582620 | -0.549619 |
| 1 | -3.926979 | 3.024740 | 0.941755  |
| 1 | -4.540724 | 2.272445 | -0.359643 |

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Cartesian coordinates of : BDC10\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.612707  | 0.066924  | 0.211571  |
| 1  | 0.247216  | 0.572854  | 1.055304  |
| 1  | 1.234615  | 0.702132  | -0.339603 |
| 1  | 1.152196  | -0.776560 | 0.513170  |
| 1  | -0.211073 | -0.219780 | -0.367758 |
| 7  | -3.810688 | -2.480595 | 0.555966  |
| 1  | -4.791674 | -2.384301 | 0.306310  |
| 1  | -3.780452 | -2.638543 | 1.559996  |
| 1  | -3.490618 | -3.343850 | 0.124263  |
| 7  | -3.389561 | 0.797295  | 1.054573  |
| 1  | -4.227417 | 1.122869  | 1.528022  |
| 1  | -3.389313 | 1.204533  | 0.120307  |
| 1  | -3.478234 | -0.211076 | 0.935949  |
| 7  | -0.686078 | 1.407989  | 2.414517  |
| 1  | -1.648608 | 1.274917  | 2.079149  |
| 1  | -0.620329 | 0.996685  | 3.341148  |
| 1  | -0.532570 | 2.405805  | 2.528162  |
| 7  | 2.148818  | -2.258405 | 1.128818  |
| 1  | 2.600688  | -2.802761 | 0.385444  |
| 1  | 1.575029  | -2.908386 | 1.659774  |
| 1  | 2.887233  | -1.954442 | 1.758340  |
| 7  | -3.541699 | 2.022331  | -2.054767 |
| 1  | -4.535938 | 1.832584  | -2.151924 |
| 1  | -3.460827 | 2.965966  | -1.684681 |
| 1  | -3.164906 | 2.055780  | -2.998679 |
| 7  | 2.364602  | 1.851043  | -1.318640 |
| 1  | 1.847943  | 2.591624  | -1.785697 |
| 1  | 2.875176  | 1.358631  | -2.046915 |
| 1  | 3.064521  | 2.309302  | -0.723692 |
| 7  | -1.788491 | -0.656508 | -1.294549 |
| 1  | -1.640211 | -1.167085 | -2.160663 |
| 1  | -2.310499 | 0.189781  | -1.530597 |
| 1  | -2.397137 | -1.230796 | -0.707933 |
| 7  | 4.535988  | 3.324558  | 0.406913  |
| 1  | 5.415130  | 2.816605  | 0.442351  |
| 1  | 4.264938  | 3.507971  | 1.368551  |
| 1  | 4.737556  | 4.225560  | -0.017435 |
| 7  | 3.608860  | -4.031918 | -1.021188 |
| 1  | 2.999958  | -4.725570 | -1.445678 |
| 1  | 4.345858  | -4.544058 | -0.544615 |
| 1  | 4.050540  | -3.525378 | -1.782874 |

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Cartesian coordinates of : BDC10\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.607718 | -0.032758 | 0.202687  |
| 1  | -0.243626 | -0.537635 | 1.047503  |
| 1  | -1.238910 | -0.663273 | -0.343411 |
| 1  | -1.136444 | 0.818217  | 0.502427  |
| 1  | 0.216349  | 0.243553  | -0.381244 |
| 7  | 3.809207  | 2.528162  | 0.506976  |
| 1  | 4.788317  | 2.427995  | 0.251531  |
| 1  | 3.786487  | 2.700462  | 1.508839  |
| 1  | 3.486159  | 3.385294  | 0.065389  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 3.394821  | -0.743504 | 1.056564  |
| 1 | 4.232951  | -1.057571 | 1.537251  |
| 1 | 3.400770  | -1.162448 | 0.127494  |
| 1 | 3.477431  | 0.263844  | 0.925602  |
| 7 | 0.691278  | -1.363404 | 2.412259  |
| 1 | 1.653741  | -1.224717 | 2.078955  |
| 1 | 0.620226  | -0.949430 | 3.337311  |
| 1 | 0.544682  | -2.361898 | 2.528876  |
| 7 | -2.100696 | 2.323637  | 1.111372  |
| 1 | -2.654138 | 2.792094  | 0.385147  |
| 1 | -1.487777 | 3.028874  | 1.512113  |
| 1 | -2.749220 | 2.060897  | 1.849166  |
| 7 | 3.558873  | -2.011502 | -2.034220 |
| 1 | 4.553396  | -1.822770 | -2.130454 |
| 1 | 3.476907  | -2.950241 | -1.652128 |
| 1 | 3.185423  | -2.057412 | -2.978936 |
| 7 | -2.390906 | -1.792096 | -1.318632 |
| 1 | -1.884267 | -2.464505 | -1.888436 |
| 1 | -2.983567 | -1.268430 | -1.957472 |
| 1 | -3.016387 | -2.332113 | -0.709546 |
| 7 | 1.792683  | 0.670625  | -1.315004 |
| 1 | 1.643165  | 1.167269  | -2.188978 |
| 1 | 2.318094  | -0.177172 | -1.537688 |
| 1 | 2.398830  | 1.256165  | -0.736964 |
| 7 | -4.350366 | -3.496109 | 0.447735  |
| 1 | -5.181960 | -2.979536 | 0.719278  |
| 1 | -3.940977 | -3.861397 | 1.302632  |
| 1 | -4.667790 | -4.297382 | -0.090502 |
| 7 | -3.851287 | 3.881090  | -0.988199 |
| 1 | -4.774577 | 3.474184  | -1.106905 |
| 1 | -3.452500 | 3.978432  | -1.917344 |
| 1 | -3.992016 | 4.821660  | -0.630272 |

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Cartesian coordinates of : BDC10\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.870964 | -0.266201 | 0.664328  |
| 1  | -0.837232 | -0.161632 | 0.843908  |
| 1  | -2.247255 | 0.560297  | 0.138868  |
| 1  | -1.949452 | -1.135743 | 0.085950  |
| 1  | -2.382278 | -0.381975 | 1.558717  |
| 7  | -5.898394 | 1.810157  | -1.720792 |
| 1  | -6.016289 | 2.402526  | -2.538037 |
| 1  | -6.210837 | 0.880830  | -1.986801 |
| 1  | -6.551817 | 2.148917  | -1.020368 |
| 7  | 0.964047  | -0.439620 | 0.915595  |
| 1  | 1.126696  | -1.210369 | 0.265110  |
| 1  | 1.586663  | 0.322158  | 0.632876  |
| 1  | 1.294397  | -0.756343 | 1.823755  |
| 7  | 3.902642  | -0.989059 | -0.736543 |
| 1  | 4.397179  | -0.822351 | -1.608351 |
| 1  | 3.575706  | -0.084600 | -0.395272 |
| 1  | 4.591089  | -1.328732 | -0.070899 |
| 7  | 2.947162  | 2.002403  | 0.210807  |
| 1  | 2.599459  | 2.547714  | 0.995767  |
| 1  | 2.624901  | 2.477383  | -0.628520 |
| 1  | 3.969811  | 2.089846  | 0.225932  |
| 7  | 1.588300  | -3.039632 | -1.101574 |
| 1  | 1.814537  | -3.860402 | -0.545063 |
| 1  | 1.549576  | -3.358916 | -2.066680 |
| 1  | 2.395929  | -2.407785 | -1.036317 |
| 7  | -1.559964 | -2.678786 | -0.898238 |
| 1  | -0.536502 | -2.751778 | -0.923113 |
| 1  | -1.913398 | -3.545286 | -0.501659 |
| 1  | -1.881766 | -2.651313 | -1.861950 |
| 7  | -2.909803 | 2.020268  | -0.800455 |
| 1  | -3.892456 | 1.910089  | -1.078032 |
| 1  | -2.851447 | 2.884350  | -0.267685 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -2.381148 | 2.178054  | -1.654642 |
| 7 | -3.341778 | -0.612531 | 3.262819  |
| 1 | -3.503830 | 0.272338  | 3.736067  |
| 1 | -2.831126 | -1.201035 | 3.915622  |
| 1 | -4.253008 | -1.044467 | 3.135062  |
| 7 | 6.082107  | 2.130634  | 0.223099  |
| 1 | 6.511899  | 1.627762  | -0.547870 |
| 1 | 6.472021  | 1.745348  | 1.078556  |
| 1 | 6.406480  | 3.091678  | 0.161757  |

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Cartesian coordinates of : BDC10\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.155676  | -0.027066 | -0.091994 |
| 1  | 0.809219  | -0.645057 | -0.850560 |
| 1  | 1.995931  | 0.532195  | -0.374955 |
| 1  | 0.332781  | 0.572735  | 0.164715  |
| 1  | 1.352177  | -0.661344 | 0.715337  |
| 7  | 1.162784  | -2.053630 | 1.969023  |
| 1  | 1.807511  | -2.833795 | 1.878808  |
| 1  | 0.219814  | -2.404251 | 1.768118  |
| 1  | 1.183547  | -1.773697 | 2.945620  |
| 7  | -0.439075 | -1.969274 | -1.551164 |
| 1  | -0.452931 | -2.267612 | -2.521871 |
| 1  | -0.281262 | -2.796447 | -0.980626 |
| 1  | -1.372463 | -1.631363 | -1.311760 |
| 7  | -3.513783 | -1.021265 | -0.781937 |
| 1  | -3.334630 | -0.177659 | -1.333719 |
| 1  | -4.179934 | -0.752954 | -0.060801 |
| 1  | -4.008905 | -1.672989 | -1.386398 |
| 7  | -1.801229 | -2.905753 | 1.254921  |
| 1  | -2.258129 | -2.847917 | 2.161610  |
| 1  | -1.923408 | -3.866285 | 0.943974  |
| 1  | -2.332272 | -2.313980 | 0.612518  |
| 7  | 3.486820  | 1.520284  | -0.867054 |
| 1  | 4.362392  | 1.012444  | -0.691806 |
| 1  | 3.487355  | 1.770126  | -1.852692 |
| 1  | 3.548987  | 2.395419  | -0.352992 |
| 7  | -1.402153 | 1.117639  | 0.509804  |
| 1  | -1.833839 | 0.305249  | 0.945111  |
| 1  | -1.918053 | 1.276519  | -0.354548 |
| 1  | -1.556049 | 1.922223  | 1.126414  |
| 7  | -2.885083 | 1.645013  | -2.481074 |
| 1  | -3.432367 | 1.372279  | -3.293873 |
| 1  | -1.954052 | 1.864505  | -2.825734 |
| 1  | -3.287460 | 2.518840  | -2.151271 |
| 7  | -1.840676 | 3.584024  | 2.434334  |
| 1  | -1.487692 | 4.454051  | 2.046205  |
| 1  | -1.348737 | 3.436306  | 3.310964  |
| 1  | -2.815615 | 3.744321  | 2.671021  |
| 7  | 6.217816  | 0.070703  | -0.385595 |
| 1  | 6.380356  | -0.205538 | 0.578417  |
| 1  | 6.966394  | 0.710709  | -0.635861 |
| 1  | 6.343651  | -0.761754 | -0.954209 |

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Cartesian coordinates of : TC10

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.724977 | 0.239533  | 0.215872  |
| 1  | 0.010313  | 0.895920  | 0.562343  |
| 1  | -1.121676 | 0.567419  | -0.690493 |
| 1  | -0.335349 | -0.712765 | 0.105404  |
| 1  | -1.558579 | 0.217442  | 0.868833  |
| 7  | 2.398122  | -0.054811 | -1.141644 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 2.164200  | 0.306859  | -2.062198 |
| 1 | 3.402748  | -0.233720 | -1.136327 |
| 1 | 2.246882  | 0.698797  | -0.474524 |
| 7 | -3.209401 | 0.040464  | 1.504547  |
| 1 | -3.869816 | 0.441446  | 0.839973  |
| 1 | -3.497622 | 0.311273  | 2.439318  |
| 1 | -3.254731 | -0.980554 | 1.427569  |
| 7 | -2.459328 | -2.894356 | 0.913724  |
| 1 | -2.397122 | -3.476808 | 1.743854  |
| 1 | -2.985167 | -3.424325 | 0.225059  |
| 1 | -1.513302 | -2.776849 | 0.552680  |
| 7 | 1.246851  | 2.141496  | 1.288465  |
| 1 | 0.923562  | 2.317672  | 2.236947  |
| 1 | 2.229909  | 1.849219  | 1.359967  |
| 1 | 1.241616  | 3.043685  | 0.818675  |
| 7 | 0.641532  | -2.412105 | -0.253474 |
| 1 | 1.363502  | -1.769319 | -0.605679 |
| 1 | 0.438651  | -3.071178 | -1.000806 |
| 1 | 1.060941  | -2.950433 | 0.500365  |
| 7 | -2.420700 | 1.132859  | -1.983529 |
| 1 | -2.285782 | 2.074240  | -2.342169 |
| 1 | -2.503729 | 0.523671  | -2.792804 |
| 1 | -3.324779 | 1.121061  | -1.504298 |
| 7 | 4.212593  | 1.207071  | 1.317843  |
| 1 | 4.378672  | 0.701055  | 2.183699  |
| 1 | 4.577373  | 0.627126  | 0.560893  |
| 1 | 4.792582  | 2.041091  | 1.357241  |
| 7 | 5.660022  | -0.594260 | -1.042958 |
| 1 | 6.394986  | -0.764707 | -0.360824 |
| 1 | 6.050848  | 0.045863  | -1.729692 |
| 1 | 5.514214  | -1.478557 | -1.523773 |
| 7 | -5.440089 | 1.201318  | -0.723811 |
| 1 | -5.988845 | 0.378776  | -0.485256 |
| 1 | -5.750914 | 1.486667  | -1.649549 |
| 1 | -5.735973 | 1.939470  | -0.089672 |

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Cartesian coordinates of : BC10\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.079035  | 0.510216  | 0.251375  |
| 1  | 0.924162  | 0.536729  | -0.355548 |
| 1  | 0.327693  | -0.151459 | 1.016050  |
| 1  | -0.123790 | 1.461161  | 0.644392  |
| 1  | -0.754765 | 0.153099  | -0.287004 |
| 7  | -0.501980 | 3.127310  | 1.383526  |
| 1  | 0.210735  | 3.425168  | 2.044750  |
| 1  | -0.587835 | 3.875066  | 0.685191  |
| 1  | -1.377371 | 3.108109  | 1.900557  |
| 7  | 2.688236  | 0.177298  | -1.050294 |
| 1  | 3.297018  | 0.989872  | -1.091999 |
| 1  | 3.126902  | -0.493282 | -0.413884 |
| 1  | 2.699162  | -0.240710 | -1.976479 |
| 7  | -2.205060 | -0.467261 | -1.193685 |
| 1  | -2.932938 | -0.799492 | -0.543277 |
| 1  | -1.986505 | -1.244998 | -1.811197 |
| 1  | -2.636385 | 0.244554  | -1.777833 |
| 7  | -6.885073 | -2.545215 | -0.917272 |
| 1  | -6.649858 | -3.313660 | -1.538406 |
| 1  | -7.330050 | -1.831730 | -1.486979 |
| 1  | -7.591468 | -2.891684 | -0.274687 |
| 7  | -4.396925 | -1.467518 | 0.713566  |
| 1  | -4.755157 | -0.747681 | 1.335000  |
| 1  | -5.192517 | -1.808747 | 0.164619  |
| 1  | -4.099514 | -2.235548 | 1.308801  |
| 7  | -0.790715 | 5.510482  | -0.635725 |
| 1  | 0.037830  | 5.688113  | -1.196045 |
| 1  | -1.567222 | 5.414972  | -1.283739 |
| 1  | -0.963793 | 6.353319  | -0.095108 |

|   |          |           |           |
|---|----------|-----------|-----------|
| 7 | 4.257897 | -1.933278 | 0.849164  |
| 1 | 4.949260 | -1.783456 | 0.104683  |
| 1 | 4.717806 | -1.675394 | 1.719322  |
| 1 | 4.108627 | -2.938542 | 0.898031  |
| 7 | 6.380162 | -1.486001 | -1.424708 |
| 1 | 6.107942 | -1.853404 | -2.331958 |
| 1 | 7.213454 | -1.995591 | -1.143681 |
| 1 | 6.665485 | -0.522150 | -1.571878 |
| 7 | 1.312379 | -1.397509 | 2.097058  |
| 1 | 2.219710 | -1.509339 | 1.638036  |
| 1 | 0.887991 | -2.318689 | 2.158726  |
| 1 | 1.489697 | -1.094284 | 3.050500  |

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Cartesian coordinates of : BCa10\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.375315 | 3.146512  | -2.203992 |
| 1  | -0.796246 | 1.837521  | -0.874477 |
| 1  | -2.387441 | 3.226618  | -2.251650 |
| 1  | -1.021460 | 4.072186  | -1.977265 |
| 1  | -1.054996 | 2.935262  | -3.145179 |
| 7  | -0.480681 | 1.181657  | -0.135112 |
| 1  | 0.096133  | 1.681773  | 0.584131  |
| 1  | -1.302486 | 0.695128  | 0.313073  |
| 1  | 0.181386  | 0.471903  | -0.511653 |
| 7  | -0.599742 | -2.619014 | -0.119462 |
| 1  | -0.096567 | -3.445834 | 0.192742  |
| 1  | 0.057601  | -2.070972 | -0.673368 |
| 1  | -1.325034 | -2.949414 | -0.750860 |
| 7  | 1.839406  | -0.528465 | -0.385636 |
| 1  | 2.555814  | 0.193759  | -0.462011 |
| 1  | 1.751623  | -0.742208 | 0.609337  |
| 1  | 2.179903  | -1.368684 | -0.860097 |
| 7  | -2.620973 | -0.346077 | 1.007388  |
| 1  | -3.514822 | -0.293455 | 0.506202  |
| 1  | -2.843321 | -0.246314 | 1.994425  |
| 1  | -2.242892 | -1.284710 | 0.875093  |
| 7  | 1.561834  | 1.953584  | 1.691421  |
| 1  | 1.515411  | 1.060581  | 2.184110  |
| 1  | 2.414139  | 1.951105  | 1.127891  |
| 1  | 1.646876  | 2.692581  | 2.382409  |
| 7  | 0.318967  | -0.902159 | 2.459200  |
| 1  | 0.677180  | -1.550736 | 3.155316  |
| 1  | -0.379681 | -0.332728 | 2.930233  |
| 1  | -0.175874 | -1.454937 | 1.756289  |
| 7  | 4.302444  | 1.772649  | -0.094615 |
| 1  | 4.499822  | 1.708775  | -1.090018 |
| 1  | 4.584746  | 2.708361  | 0.186914  |
| 1  | 4.939682  | 1.130654  | 0.369899  |
| 7  | -5.486406 | -0.234654 | -0.304089 |
| 1  | -5.997484 | -1.033146 | 0.061953  |
| 1  | -5.580715 | -0.267874 | -1.314991 |
| 1  | -5.982771 | 0.595068  | 0.008436  |
| 7  | 2.504764  | -3.293512 | -1.816731 |
| 1  | 2.897976  | -3.991758 | -1.191584 |
| 1  | 3.217500  | -3.101388 | -2.515660 |
| 1  | 1.735903  | -3.740758 | -2.308242 |

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Cartesian coordinates of : BDC10\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.153623 | 0.662217  | -1.186472 |
| 1  | -1.353286 | -0.356178 | -0.965979 |
| 1  | -1.598986 | 1.297952  | -0.484880 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.109856 | 0.734615  | -1.160583 |
| 1 | -1.502523 | 0.894537  | -2.133903 |
| 7 | 1.699417  | 0.222889  | -1.096298 |
| 1 | 2.388708  | 0.780148  | -0.590389 |
| 1 | 1.660608  | -0.690162 | -0.636831 |
| 1 | 2.089959  | 0.061678  | -2.021398 |
| 7 | -1.251580 | -2.108087 | -0.634339 |
| 1 | -1.898496 | -2.480286 | 0.068062  |
| 1 | -1.371584 | -2.678787 | -1.467254 |
| 1 | -0.296242 | -2.268344 | -0.303272 |
| 7 | -2.196762 | 1.317947  | -3.939121 |
| 1 | -3.199562 | 1.163907  | -4.001946 |
| 1 | -1.769619 | 0.741348  | -4.659023 |
| 1 | -2.034205 | 2.284694  | -4.207617 |
| 7 | -2.494261 | 2.479969  | 0.672736  |
| 1 | -3.491715 | 2.282729  | 0.688326  |
| 1 | -2.172065 | 2.437586  | 1.646275  |
| 1 | -2.403077 | 3.448847  | 0.377992  |
| 7 | 4.450136  | -1.115543 | 0.462395  |
| 1 | 4.268848  | -0.117410 | 0.362105  |
| 1 | 5.005559  | -1.245499 | 1.302983  |
| 1 | 5.034187  | -1.396835 | -0.319911 |
| 7 | -1.649077 | 2.480449  | 3.699418  |
| 1 | -1.218652 | 3.364769  | 3.954253  |
| 1 | -1.008252 | 1.747160  | 3.987912  |
| 1 | -2.481582 | 2.386349  | 4.274274  |
| 7 | 1.768192  | -2.704380 | 0.397092  |
| 1 | 2.691279  | -2.264387 | 0.490702  |
| 1 | 1.909182  | -3.573553 | -0.111710 |
| 1 | 1.473707  | -2.969174 | 1.333693  |
| 7 | -3.331165 | -3.435508 | 1.358753  |
| 1 | -4.278634 | -3.310233 | 1.014345  |
| 1 | -3.326466 | -3.121780 | 2.324721  |
| 1 | -3.155876 | -4.436125 | 1.374850  |
| 7 | 4.074108  | 2.165164  | 0.157017  |
| 1 | 3.478838  | 2.945471  | -0.109026 |
| 1 | 4.925664  | 2.256130  | -0.391305 |
| 1 | 4.336436  | 2.324999  | 1.126261  |

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Cartesian coordinates of : BC10\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.769763 | 0.203302  | -0.669968 |
| 1  | -1.164426 | 0.296771  | -1.622740 |
| 1  | -0.235661 | 1.074479  | -0.427400 |
| 1  | -1.558758 | 0.055508  | 0.029576  |
| 1  | -0.120649 | -0.613000 | -0.640218 |
| 7  | -2.854258 | -0.187292 | 1.210296  |
| 1  | -3.487712 | 0.617595  | 1.253175  |
| 1  | -3.424993 | -1.017806 | 1.023515  |
| 1  | -2.478067 | -0.303399 | 2.148130  |
| 7  | -1.945252 | 0.510928  | -3.435971 |
| 1  | -1.692031 | 1.400467  | -3.857387 |
| 1  | -1.657806 | -0.212619 | -4.089159 |
| 1  | -2.960601 | 0.484137  | -3.399484 |
| 7  | 3.455296  | 1.037965  | -0.790803 |
| 1  | 4.147738  | 0.933050  | -0.049643 |
| 1  | 3.138872  | 0.096981  | -1.011910 |
| 1  | 3.936435  | 1.397948  | -1.609817 |
| 7  | -4.811536 | 2.306106  | 1.512935  |
| 1  | -5.243445 | 2.230275  | 2.429426  |
| 1  | -4.348595 | 3.209624  | 1.481131  |
| 1  | -5.567603 | 2.339630  | 0.835450  |
| 7  | 0.858689  | 2.505014  | -0.027038 |
| 1  | 1.795760  | 2.138876  | -0.238943 |
| 1  | 0.728477  | 3.352629  | -0.571950 |
| 1  | 0.849703  | 2.784416  | 0.949835  |
| 7  | 0.994554  | -2.165454 | -0.523757 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.003408  | -2.710421 | -1.382190 |
| 1 | 1.975426  | -2.012965 | -0.263906 |
| 1 | 0.595937  | -2.770453 | 0.190079  |
| 7 | -4.681167 | -2.769635 | 0.805608  |
| 1 | -4.542112 | -3.347922 | -0.017640 |
| 1 | -5.651061 | -2.467559 | 0.791484  |
| 1 | -4.577536 | -3.378217 | 1.612463  |
| 7 | 4.061003  | -1.950629 | 0.210587  |
| 1 | 4.455870  | -1.150287 | 0.706790  |
| 1 | 4.668069  | -2.127107 | -0.585917 |
| 1 | 4.153394  | -2.757569 | 0.822112  |
| 7 | 5.628953  | 0.561835  | 1.672661  |
| 1 | 5.492112  | 1.541941  | 1.907161  |
| 1 | 6.563159  | 0.487906  | 1.278070  |
| 1 | 5.651066  | 0.062127  | 2.558054  |

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Cartesian coordinates of : BL10\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.725897 | 0.000106  | 0.082238  |
| 1  | -0.717892 | 0.855481  | 0.684833  |
| 1  | -1.489183 | 0.076810  | -0.628630 |
| 1  | 0.199845  | -0.090264 | -0.407984 |
| 1  | -0.886868 | -0.841049 | 0.683057  |
| 7  | 1.824290  | -0.245000 | -1.271640 |
| 1  | 1.933507  | 0.428939  | -2.025119 |
| 1  | 2.614404  | -0.099309 | -0.626654 |
| 1  | 1.954866  | -1.161753 | -1.691550 |
| 7  | -0.669844 | 2.357477  | 1.821907  |
| 1  | 0.196430  | 2.376063  | 2.353908  |
| 1  | -0.731787 | 3.254757  | 1.327711  |
| 1  | -1.422489 | 2.346994  | 2.505331  |
| 7  | -1.164385 | -2.319436 | 1.821591  |
| 1  | -1.098317 | -3.225956 | 1.345065  |
| 1  | -2.078382 | -2.288078 | 2.265759  |
| 1  | -0.482924 | -2.335899 | 2.576015  |
| 7  | 4.241863  | 0.169835  | 0.598424  |
| 1  | 4.281829  | -0.490989 | 1.369331  |
| 1  | 4.296936  | 1.095967  | 1.012863  |
| 1  | 5.098018  | 0.039369  | 0.050188  |
| 7  | -0.983112 | -5.174636 | 0.515470  |
| 1  | -0.030759 | -5.456666 | 0.302183  |
| 1  | -1.341486 | -5.844828 | 1.189946  |
| 1  | -1.523130 | -5.299057 | -0.335850 |
| 7  | -2.823324 | 0.220944  | -1.956871 |
| 1  | -2.766156 | 1.111753  | -2.443587 |
| 1  | -2.720157 | -0.497785 | -2.668569 |
| 1  | -3.780416 | 0.143274  | -1.594799 |
| 7  | -0.835044 | 5.188498  | 0.461606  |
| 1  | -0.637095 | 5.881039  | 1.178352  |
| 1  | -0.163071 | 5.340025  | -0.284982 |
| 1  | -1.750045 | 5.414691  | 0.082713  |
| 7  | -5.814399 | 0.012581  | -1.005322 |
| 1  | -6.404793 | 0.269151  | -1.791537 |
| 1  | -6.062154 | 0.632009  | -0.239281 |
| 1  | -6.091809 | -0.923917 | -0.726007 |
| 7  | 6.926196  | -0.206200 | -1.038084 |
| 1  | 7.027894  | 0.471252  | -1.788010 |
| 1  | 7.016478  | -1.126374 | -1.458480 |
| 1  | 7.724298  | -0.084816 | -0.421444 |

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Cartesian coordinates of : BL10\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 0.070967  | 0.736611  | 0.362433  |
| 1 | -0.530962 | 1.357003  | -0.230686 |
| 1 | 0.313705  | 1.218795  | 1.246676  |
| 1 | -0.466914 | -0.143230 | 0.575791  |
| 1 | 0.954553  | 0.496760  | -0.158712 |
| 7 | -1.473205 | -1.644923 | 0.880729  |
| 1 | -1.685647 | -1.801835 | 1.862537  |
| 1 | -2.375254 | -1.583116 | 0.387233  |
| 1 | -1.015255 | -2.490947 | 0.551511  |
| 7 | -1.696213 | 2.308857  | -1.333626 |
| 1 | -2.611766 | 1.868160  | -1.291255 |
| 1 | -1.830725 | 3.300500  | -1.105917 |
| 1 | -1.405665 | 2.269687  | -2.307207 |
| 7 | 2.488322  | 0.083284  | -1.070456 |
| 1 | 3.227693  | -0.269657 | -0.445228 |
| 1 | 2.878623  | 0.883277  | -1.562139 |
| 1 | 2.335617  | -0.633653 | -1.775271 |
| 7 | -4.198887 | -1.549918 | -0.570739 |
| 1 | -4.644212 | -2.449917 | -0.362776 |
| 1 | -4.150361 | -1.475317 | -1.583093 |
| 1 | -4.842427 | -0.827744 | -0.259173 |
| 7 | 4.753915  | -0.991396 | 0.717968  |
| 1 | 5.190849  | -0.293483 | 1.313507  |
| 1 | 4.486316  | -1.759961 | 1.326459  |
| 1 | 5.485903  | -1.346921 | 0.094449  |
| 7 | 7.062508  | -2.080031 | -1.150335 |
| 1 | 6.789838  | -2.881993 | -1.710826 |
| 1 | 7.409907  | -1.375339 | -1.794090 |
| 1 | 7.851420  | -2.373402 | -0.581521 |
| 7 | -2.190349 | 5.366873  | -0.807906 |
| 1 | -2.792580 | 5.702415  | -1.554464 |
| 1 | -2.659951 | 5.586046  | 0.065844  |
| 1 | -1.346957 | 5.932445  | -0.837518 |
| 7 | -5.631419 | -4.300881 | 0.034689  |
| 1 | -5.523241 | -4.332483 | -0.450833 |
| 1 | -5.829160 | -4.438164 | 1.021500  |
| 1 | -5.099977 | -5.109528 | -0.274132 |
| 7 | 0.826731  | 2.097014  | 2.941828  |
| 1 | 0.063060  | 2.150738  | 3.610222  |
| 1 | 1.155116  | 3.047725  | 2.796404  |
| 1 | 1.581859  | 1.594717  | 3.400616  |

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Cartesian coordinates of : BC10\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.586975  | 0.034685  | -0.151174 |
| 1  | -0.455284 | 0.036894  | -0.357880 |
| 1  | 1.034347  | 0.906851  | -0.512502 |
| 1  | 0.647840  | -0.003099 | 0.884861  |
| 1  | 1.044161  | -0.803124 | -0.575786 |
| 7  | 0.113255  | -0.071207 | 2.761177  |
| 1  | 0.405998  | 0.735155  | 3.305806  |
| 1  | -0.909768 | -0.094027 | 2.780757  |
| 1  | 0.441535  | -0.893109 | 3.260361  |
| 7  | -2.231444 | 0.025707  | -0.268949 |
| 1  | -2.686581 | 0.872203  | -0.621768 |
| 1  | -2.684333 | -0.777050 | -0.714648 |
| 1  | -2.425137 | -0.030273 | 0.729970  |
| 7  | 1.835173  | -2.310063 | -1.405172 |
| 1  | 1.136012  | -3.020861 | -1.604048 |
| 1  | 2.568583  | -2.763947 | -0.849270 |
| 1  | 2.254175  | -2.066439 | -2.298930 |
| 7  | 1.801154  | 2.485544  | -1.221827 |
| 1  | 1.132942  | 3.251583  | -1.204598 |
| 1  | 2.637464  | 2.811009  | -0.724110 |
| 1  | 2.068493  | 2.364189  | -2.195219 |
| 7  | 4.109331  | -3.808997 | 0.168838  |
| 1  | 4.509283  | -4.503926 | -0.455326 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 4.873653  | -3.211370 | 0.469613  |
| 1 | 3.785543  | -4.307929 | 0.992328  |
| 7 | 4.378207  | 3.601678  | 0.192293  |
| 1 | 5.152812  | 2.944835  | 0.212544  |
| 1 | 4.230669  | 3.910877  | 1.148593  |
| 1 | 4.695529  | 4.412398  | -0.331625 |
| 7 | -3.114959 | -0.152451 | 3.035993  |
| 1 | -3.077792 | -0.202182 | 4.051035  |
| 1 | -3.645834 | -0.963620 | 2.729525  |
| 1 | -3.675734 | 0.665095  | 2.810449  |
| 7 | -3.710232 | -2.417704 | -1.729195 |
| 1 | -3.409634 | -2.453618 | -2.698844 |
| 1 | -4.711228 | -2.245033 | -1.739652 |
| 1 | -3.577506 | -3.348718 | -1.345584 |
| 7 | -3.716314 | 2.620532  | -1.432750 |
| 1 | -3.442079 | 2.754470  | -2.401625 |
| 1 | -3.555951 | 3.503513  | -0.957149 |
| 1 | -4.720199 | 2.465196  | -1.431917 |

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Cartesian coordinates of : BC10\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.249344  | 0.033594  | 0.816183  |
| 1  | -0.331304 | 0.819640  | 0.439193  |
| 1  | -0.055359 | -0.804713 | 0.264188  |
| 1  | 1.283161  | 0.227068  | 0.672529  |
| 1  | 0.059118  | -0.106145 | 1.822889  |
| 7  | -3.385065 | -0.253670 | -2.450256 |
| 1  | -4.215189 | 0.075818  | -1.964389 |
| 1  | -3.268862 | 0.344175  | -3.264388 |
| 1  | -3.611246 | -1.178887 | -2.806620 |
| 7  | -0.895546 | -1.917787 | -0.970847 |
| 1  | -0.273310 | -2.183516 | -1.729380 |
| 1  | -1.640989 | -1.355418 | -1.384112 |
| 1  | -1.314465 | -2.782163 | -0.614603 |
| 7  | -1.538246 | 1.811423  | -0.593675 |
| 1  | -2.224613 | 2.391896  | -0.102163 |
| 1  | -1.064702 | 2.414931  | -1.260347 |
| 1  | -2.047168 | 1.111999  | -1.135313 |
| 7  | -0.224641 | -0.355242 | 3.783989  |
| 1  | 0.073235  | 0.457471  | 4.316527  |
| 1  | -1.199614 | -0.517852 | 4.019706  |
| 1  | 0.299515  | -1.147974 | 4.144025  |
| 7  | 4.776851  | -1.927362 | -0.474583 |
| 1  | 4.500904  | -2.832867 | -0.106771 |
| 1  | 5.728280  | -1.759979 | -0.160184 |
| 1  | 4.813942  | -2.018404 | -1.485511 |
| 7  | 3.026409  | 0.558780  | 0.484800  |
| 1  | 3.454169  | 0.823680  | 1.368723  |
| 1  | 3.545635  | -0.257854 | 0.147572  |
| 1  | 3.211676  | 1.329310  | -0.164855 |
| 7  | -2.103808 | -4.684977 | 0.026701  |
| 1  | -2.965788 | -4.625182 | 0.560712  |
| 1  | -1.433055 | -5.179786 | 0.607353  |
| 1  | -2.295197 | -5.282475 | -0.772373 |
| 7  | -3.589259 | 3.752548  | 0.858461  |
| 1  | -4.310116 | 3.317257  | 1.426463  |
| 1  | -4.065941 | 4.337479  | 0.178164  |
| 1  | -3.072787 | 4.378028  | 1.470117  |
| 7  | 3.781185  | 3.002169  | -1.421708 |
| 1  | 3.562688  | 2.879522  | -2.405935 |
| 1  | 4.790717  | 3.094128  | -1.354447 |
| 1  | 3.386100  | 3.894475  | -1.140227 |

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Cartesian coordinates of : BC10\_5

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## Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.002055  | 0.089343  | 0.009870  |
| 1  | -0.075292 | 0.720284  | 0.826646  |
| 1  | -0.862160 | -0.521158 | -0.071961 |
| 1  | 0.081297  | 0.722223  | -0.806381 |
| 1  | 0.863919  | -0.524498 | 0.091145  |
| 7  | 0.198276  | 2.379508  | -1.882140 |
| 1  | -0.548085 | 2.480487  | -2.563941 |
| 1  | 0.131473  | 3.168382  | -1.237349 |
| 1  | 1.073888  | 2.474500  | -2.388568 |
| 7  | -0.191756 | 2.406524  | 1.875351  |
| 1  | -1.069554 | 2.520920  | 2.373681  |
| 1  | 0.551948  | 2.529815  | 2.556200  |
| 1  | -0.120242 | 3.169132  | 1.201027  |
| 7  | 2.258458  | -1.632378 | 0.221503  |
| 1  | 3.090529  | -1.217179 | 0.651420  |
| 1  | 2.537006  | -2.000213 | -0.693567 |
| 1  | 2.015378  | -2.438844 | 0.791649  |
| 7  | -2.262030 | -1.622228 | -0.200659 |
| 1  | -2.555652 | -1.971582 | 0.716941  |
| 1  | -3.085076 | -1.209110 | -0.649541 |
| 1  | -2.016710 | -2.440451 | -0.752809 |
| 7  | 3.138829  | -2.904030 | -2.568060 |
| 1  | 3.429610  | -3.862334 | -2.397334 |
| 1  | 2.421403  | -2.938131 | -3.286096 |
| 1  | 3.937142  | -2.423434 | -2.972368 |
| 7  | -4.896823 | -0.556992 | -1.656632 |
| 1  | -4.780271 | -0.349966 | -2.644113 |
| 1  | -5.348382 | 0.250236  | -1.237206 |
| 1  | -5.556107 | -1.327481 | -1.594612 |
| 7  | 0.019925  | 5.116286  | -0.023611 |
| 1  | 0.062169  | 5.570586  | -0.932954 |
| 1  | 0.819560  | 5.463331  | 0.500435  |
| 1  | -0.807783 | 5.487822  | 0.436157  |
| 7  | 4.920921  | -0.562185 | 1.622626  |
| 1  | 5.575749  | -1.336281 | 1.558423  |
| 1  | 4.819808  | -0.345130 | 2.609659  |
| 1  | 5.369815  | 0.238818  | 1.188665  |
| 7  | -3.188283 | -2.839307 | 2.598469  |
| 1  | -3.473107 | -3.801669 | 2.441034  |
| 1  | -3.995281 | -2.353626 | 2.978737  |
| 1  | -2.483996 | -2.857238 | 3.329968  |

Cartesian coordinates of : BDC10\_6

## Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.347887  | 0.085078  | -1.521913 |
| 1  | 0.857438  | 0.048294  | -0.556608 |
| 1  | 0.607586  | 0.948426  | -2.028341 |
| 1  | 0.621806  | -0.733822 | -2.091135 |
| 1  | -0.685725 | 0.070270  | -1.357561 |
| 7  | -3.330559 | -2.636620 | 0.714996  |
| 1  | -4.056426 | -2.472870 | 1.407835  |
| 1  | -2.685320 | -3.308957 | 1.121448  |
| 1  | -3.781475 | -3.109882 | -0.063841 |
| 7  | -1.514536 | -0.109973 | 2.018198  |
| 1  | -1.692002 | -0.166646 | 3.016786  |
| 1  | -1.986738 | 0.723133  | 1.671217  |
| 1  | -1.972222 | -0.908099 | 1.581245  |
| 7  | 1.469592  | -0.029119 | 0.975175  |
| 1  | 0.608961  | -0.064256 | 1.529507  |
| 1  | 2.020563  | -0.864136 | 1.189055  |
| 1  | 2.013290  | 0.781914  | 1.280850  |
| 7  | 1.237770  | -2.310223 | -3.153722 |
| 1  | 0.478362  | -2.846411 | -3.564011 |
| 1  | 1.753152  | -2.944826 | -2.549977 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.862430  | -2.060033 | -3.915240 |
| 7 | -3.374919 | 2.507672  | 0.985883  |
| 1 | -4.118502 | 2.254009  | 1.631236  |
| 1 | -2.753386 | 3.135471  | 1.489023  |
| 1 | -3.809670 | 3.063821  | 0.254061  |
| 7 | 1.167586  | 2.589574  | -3.028708 |
| 1 | 2.164671  | 2.755603  | -2.923383 |
| 1 | 0.695544  | 3.420861  | -2.684196 |
| 1 | 0.982584  | 2.542038  | -4.026849 |
| 7 | -2.534446 | 0.038511  | -0.992077 |
| 1 | -3.131311 | 0.077968  | -1.813669 |
| 1 | -2.790109 | 0.828777  | -0.396302 |
| 1 | -2.778865 | -0.813579 | -0.482990 |
| 7 | 3.273255  | 2.403080  | 2.088226  |
| 1 | 2.968699  | 3.360527  | 1.940836  |
| 1 | 4.233441  | 2.345616  | 1.762202  |
| 1 | 3.293874  | 2.252967  | 3.092685  |
| 7 | 3.318155  | -2.532904 | 1.839645  |
| 1 | 3.380369  | -2.402922 | 2.845276  |
| 1 | 4.262916  | -2.458062 | 1.474401  |
| 1 | 3.017573  | -3.490721 | 1.686514  |

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Cartesian coordinates of : BTC10\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.006733 | 0.629368  | 0.253167  |
| 1  | -0.835833 | 1.152612  | -0.107999 |
| 1  | -0.014789 | 0.638093  | 1.295802  |
| 1  | -0.030275 | -0.363744 | -0.075792 |
| 1  | 0.867429  | 1.086007  | -0.067088 |
| 7  | -3.072158 | -0.816646 | -1.020972 |
| 1  | -3.866591 | -1.278571 | -0.566973 |
| 1  | -3.305923 | -0.740596 | -2.007505 |
| 1  | -3.013948 | 0.133999  | -0.663137 |
| 7  | 2.737785  | 1.622763  | -0.435493 |
| 1  | 3.333527  | 2.243220  | 0.107210  |
| 1  | 3.072425  | 1.671937  | -1.394695 |
| 1  | 2.917313  | 0.664280  | -0.102377 |
| 7  | 2.683214  | -1.269827 | 0.530497  |
| 1  | 3.472146  | -1.765490 | 0.101143  |
| 1  | 2.737564  | -1.452898 | 1.528763  |
| 1  | 1.827021  | -1.708689 | 0.196432  |
| 7  | -2.114139 | 2.420893  | -0.710180 |
| 1  | -2.498263 | 2.366092  | -1.650172 |
| 1  | -2.862703 | 2.759134  | -0.111144 |
| 1  | -1.381699 | 3.142217  | -0.727815 |
| 7  | -0.372539 | -2.126837 | -0.635825 |
| 1  | -1.351950 | -1.856822 | -0.817004 |
| 1  | -0.392750 | -2.929139 | -0.011407 |
| 1  | 0.017523  | -2.455311 | -1.515678 |
| 7  | 0.494608  | 4.033556  | -0.707858 |
| 1  | 0.626587  | 4.536812  | -1.580805 |
| 1  | 0.625628  | 4.710700  | 0.038125  |
| 1  | 1.246328  | 3.348429  | -0.635391 |
| 7  | -5.577042 | -2.331321 | 0.173829  |
| 1  | -5.668252 | -2.380559 | 1.184239  |
| 1  | -6.433153 | -1.911576 | -0.177010 |
| 1  | -5.560554 | -3.288871 | -0.165392 |
| 7  | 0.024299  | 0.654695  | 3.209064  |
| 1  | -0.532893 | 1.406121  | 3.607330  |
| 1  | 0.970931  | 0.779446  | 3.558433  |
| 1  | -0.324455 | -0.209823 | 3.614689  |
| 7  | 5.183607  | -2.748732 | -0.705866 |
| 1  | 5.240737  | -2.729189 | -1.719917 |
| 1  | 5.217647  | -3.725944 | -0.429933 |
| 1  | 6.034917  | -2.317256 | -0.357465 |

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Cartesian coordinates of : BL10\_3

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.499017  | 0.100044  | 0.330951  |
| 1  | 0.965915  | -0.632994 | -0.245887 |
| 1  | -0.568025 | 0.075069  | 0.152402  |
| 1  | 0.682687  | -0.075877 | 1.332926  |
| 1  | 0.871740  | 1.039032  | 0.070116  |
| 7  | 0.933323  | -0.389654 | 3.294385  |
| 1  | 0.028631  | -0.446478 | 3.753758  |
| 1  | 1.421492  | -1.256932 | 3.498861  |
| 1  | 1.450705  | 0.353699  | 3.755012  |
| 7  | 1.732851  | -1.953180 | -1.392803 |
| 1  | 2.256504  | -1.519967 | -2.148888 |
| 1  | 2.362220  | -2.630422 | -0.948911 |
| 1  | 0.988166  | -2.488019 | -1.832269 |
| 7  | 1.452343  | 2.784936  | -0.437158 |
| 1  | 2.462546  | 2.954276  | -0.380452 |
| 1  | 1.002918  | 3.496116  | 0.133626  |
| 1  | 1.175855  | 2.976364  | -1.396601 |
| 7  | -3.989461 | 1.836700  | 1.913891  |
| 1  | -3.573105 | 2.689605  | 2.275100  |
| 1  | -4.341826 | 1.318867  | 2.713388  |
| 1  | -4.797949 | 2.113987  | 1.364906  |
| 7  | 4.526046  | 3.464161  | -0.316125 |
| 1  | 4.649188  | 4.375201  | 0.116521  |
| 1  | 5.109098  | 2.812695  | 0.200850  |
| 1  | 4.918307  | 3.530596  | -1.250964 |
| 7  | -2.239395 | 0.043485  | -0.130903 |
| 1  | -2.620888 | -0.905025 | -0.079202 |
| 1  | -2.753747 | 0.611933  | 0.547405  |
| 1  | -2.466822 | 0.407775  | -1.060234 |
| 7  | 3.714552  | -4.117847 | -0.230542 |
| 1  | 4.084753  | -4.620973 | -1.032008 |
| 1  | 4.513067  | -3.743262 | 0.273345  |
| 1  | 3.284027  | -4.810630 | 0.374940  |
| 7  | -3.079155 | 1.158899  | -3.044847 |
| 1  | -4.007509 | 0.784445  | -3.217448 |
| 1  | -2.498460 | 0.878489  | -3.829341 |
| 1  | -3.158880 | 2.170636  | -3.083571 |
| 7  | -3.569502 | -2.897916 | 0.001561  |
| 1  | -4.512717 | -2.759392 | 0.352222  |
| 1  | -3.134591 | -3.597954 | 0.594822  |
| 1  | -3.657632 | -3.308259 | -0.923298 |

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Cartesian coordinates of : BL10\_4

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.205024 | -0.136305 | 0.960459  |
| 1  | -1.032108 | -0.049011 | 0.308254  |
| 1  | -0.244772 | 0.612607  | 1.671751  |
| 1  | -0.240124 | -1.054301 | 1.434668  |
| 1  | 0.717715  | -0.056933 | 0.402439  |
| 7  | -0.282473 | -2.855882 | 2.307785  |
| 1  | -0.455598 | -2.836160 | 3.308783  |
| 1  | -1.005755 | -3.439236 | 1.896640  |
| 1  | 0.599737  | -3.341448 | 2.171636  |
| 7  | -2.429599 | 0.082977  | -0.838782 |
| 1  | -2.082873 | 0.123581  | -1.793958 |
| 1  | -3.068551 | -0.716257 | -0.795945 |
| 1  | -2.991690 | 0.927630  | -0.698421 |
| 7  | 2.173327  | 0.054471  | -0.466639 |
| 1  | 2.991651  | 0.057968  | 0.148313  |
| 1  | 2.216352  | 0.909906  | -1.027290 |
| 1  | 2.286821  | -0.731596 | -1.112491 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 2.621760  | -2.360599 | -2.567905 |
| 1 | 3.216771  | -1.978204 | -3.296949 |
| 1 | 1.789491  | -2.720041 | -3.025404 |
| 1 | 3.112673  | -3.159205 | -2.177216 |
| 7 | 4.853497  | 0.086288  | 1.340554  |
| 1 | 4.868716  | -0.402687 | 2.230410  |
| 1 | 5.566090  | -0.342193 | 0.757075  |
| 1 | 5.156615  | 1.038504  | 1.522095  |
| 7 | -0.293902 | 2.065290  | 3.054594  |
| 1 | -1.209846 | 2.177101  | 3.480008  |
| 1 | 0.364847  | 1.909856  | 3.812488  |
| 1 | -0.052759 | 2.959530  | 2.636613  |
| 7 | -4.549144 | -2.322485 | -0.878640 |
| 1 | -5.249694 | -2.001458 | -1.540788 |
| 1 | -4.221145 | -3.222967 | -1.214979 |
| 1 | -5.032162 | -2.493145 | -0.001608 |
| 7 | -4.290387 | 2.677070  | -0.574773 |
| 1 | -3.827727 | 3.579182  | -0.514966 |
| 1 | -4.939432 | 2.626439  | 0.204891  |
| 1 | -4.850851 | 2.691355  | -1.422019 |
| 7 | 2.423685  | 2.701903  | -2.301916 |
| 1 | 2.548516  | 3.573197  | -1.795444 |
| 1 | 1.656110  | 2.844816  | -2.951264 |
| 1 | 3.260809  | 2.564084  | -2.860477 |

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Cartesian coordinates of : BC10\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -4.754407 | -1.077505 | -0.997179 |
| 1  | -3.037744 | -0.705643 | 0.018015  |
| 1  | -4.664506 | -1.806829 | -1.699335 |
| 1  | -5.475946 | -1.389828 | -0.339005 |
| 1  | -5.129620 | -0.264458 | -1.477965 |
| 7  | -7.045248 | -2.054516 | 0.948433  |
| 1  | -6.835863 | -2.936728 | 1.406233  |
| 1  | -7.272990 | -1.389351 | 1.681483  |
| 1  | -7.893326 | -2.198010 | 0.407806  |
| 7  | -2.155283 | -0.511398 | 0.516642  |
| 1  | -1.894509 | -1.365635 | 1.002435  |
| 1  | -0.920739 | 0.070105  | -0.625582 |
| 1  | -2.365984 | 0.173793  | 1.237745  |
| 7  | 0.727774  | 2.945846  | -0.825978 |
| 1  | 1.666077  | 2.734122  | -0.466714 |
| 1  | 0.847501  | 3.534082  | -1.646735 |
| 1  | 0.233616  | 3.512924  | -0.128888 |
| 7  | -0.233692 | 0.422757  | -1.353605 |
| 1  | 0.071260  | 1.444156  | -1.145297 |
| 1  | -0.685841 | 0.387365  | -2.265004 |
| 1  | 0.629983  | -0.175457 | -1.380979 |
| 7  | 3.528520  | 1.968572  | 0.179595  |
| 1  | 3.558815  | 0.968189  | 0.376165  |
| 1  | 4.277718  | 2.169325  | -0.476824 |
| 1  | 3.764580  | 2.450584  | 1.042500  |
| 7  | 4.025053  | -1.151160 | 1.120486  |
| 1  | 4.978170  | -0.807047 | 1.211568  |
| 1  | 3.595057  | -1.039676 | 2.035383  |
| 1  | 4.102687  | -2.161067 | 0.953839  |
| 7  | 2.242975  | -1.069493 | -1.499444 |
| 1  | 2.167198  | -2.058199 | -1.724231 |
| 1  | 2.818004  | -0.653984 | -2.228290 |
| 1  | 2.781847  | -1.007125 | -0.629482 |
| 7  | 4.407906  | -4.235427 | 0.586920  |
| 1  | 5.025068  | -4.554898 | 1.328580  |
| 1  | 4.886490  | -4.423167 | -0.289444 |
| 1  | 3.590692  | -4.838406 | 0.610580  |
| 7  | -0.755043 | 4.886173  | 1.181734  |
| 1  | -0.232598 | 5.757343  | 1.158029  |
| 1  | -0.800748 | 4.599645  | 2.155134  |

1      -1.704245      5.106927      0.895049

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Cartesian coordinates of :      BC10\_7

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.135310  | 0.336559  | 0.517771  |
| 1  | 0.596375  | 1.117473  | 0.014785  |
| 1  | 1.428299  | 0.654404  | 1.438936  |
| 1  | 0.432551  | -0.439592 | 0.617329  |
| 1  | 1.992563  | 0.022829  | -0.033769 |
| 7  | -1.124195 | -1.410137 | 0.530939  |
| 1  | -1.492240 | -1.759770 | 1.411638  |
| 1  | -1.825340 | -0.763364 | 0.156640  |
| 1  | -1.088626 | -2.206022 | -0.100493 |
| 7  | -0.573642 | 2.108608  | -0.762141 |
| 1  | -1.458481 | 1.598658  | -0.691425 |
| 1  | -0.705610 | 3.035587  | -0.341779 |
| 1  | -0.393331 | 2.256156  | -1.751748 |
| 7  | 3.438131  | -0.478487 | -0.887420 |
| 1  | 4.248714  | -0.495708 | -0.247475 |
| 1  | 3.680796  | 0.143469  | -1.654641 |
| 1  | 3.360664  | -1.409098 | -1.290202 |
| 7  | -3.427746 | 0.547413  | -0.551565 |
| 1  | -3.934526 | -0.277509 | -0.200450 |
| 1  | -3.664247 | 0.633099  | -1.537201 |
| 1  | -3.841378 | 1.354697  | -0.091048 |
| 7  | 5.833028  | -0.529271 | 1.000792  |
| 1  | 6.102141  | 0.385794  | 1.351791  |
| 1  | 5.709777  | -1.122519 | 1.816759  |
| 1  | 6.640658  | -0.897719 | 0.487260  |
| 7  | 8.361851  | -1.658929 | -0.513999 |
| 1  | 8.280042  | -2.644995 | -0.743722 |
| 1  | 8.570814  | -1.171352 | -1.380198 |
| 1  | 9.179138  | -1.563129 | 0.081775  |
| 7  | -0.921366 | 4.997466  | 0.432693  |
| 1  | -1.567992 | 5.529102  | -0.143255 |
| 1  | -1.274413 | 5.041344  | 1.384283  |
| 1  | -0.040727 | 5.504139  | 0.424482  |
| 7  | -4.792745 | -1.997763 | 0.545984  |
| 1  | -5.777484 | -1.954593 | 0.262210  |
| 1  | -4.786312 | -2.083962 | 1.558728  |
| 1  | -4.422232 | -2.871017 | 0.181134  |
| 7  | -7.834260 | -1.903041 | -0.289336 |
| 1  | -8.364031 | -1.240903 | 0.269912  |
| 1  | -8.265739 | -2.812766 | -0.154257 |
| 1  | -7.980388 | -1.649655 | -1.262017 |

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Cartesian coordinates of :      BL10\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.014404 | -0.204637 | -0.666636 |
| 1  | 0.001173  | 0.824640  | -0.935489 |
| 1  | 0.859526  | -0.455824 | -0.112730 |
| 1  | -0.890199 | -0.426896 | -0.103548 |
| 1  | -0.028220 | -0.763834 | -1.517464 |
| 7  | -2.366649 | -0.830028 | 0.774903  |
| 1  | -2.891790 | -0.004846 | 1.053317  |
| 1  | -2.995291 | -1.402718 | 0.189381  |
| 1  | -2.194557 | -1.357704 | 1.627000  |
| 7  | 0.146613  | 7.392127  | 0.015692  |
| 1  | 0.322855  | 8.019203  | 0.795302  |
| 1  | 0.846199  | 7.598435  | -0.691228 |
| 1  | -0.753023 | 7.655748  | -0.375389 |
| 7  | 0.223944  | 4.396621  | 1.015771  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.197450  | 5.362691  | 0.673029  |
| 1 | 1.084354  | 4.296943  | 1.547299  |
| 1 | -0.535967 | 4.300747  | 1.683666  |
| 7 | -4.224489 | -2.524748 | -0.960231 |
| 1 | -3.807743 | -3.386904 | -1.300705 |
| 1 | -4.577559 | -2.036537 | -1.778751 |
| 1 | -5.041226 | -2.792688 | -0.401016 |
| 7 | 6.612752  | -3.677735 | 0.656139  |
| 1 | 7.158346  | -4.311135 | 0.078865  |
| 1 | 7.222554  | -2.902550 | 0.898914  |
| 1 | 6.406464  | -4.171284 | 1.519601  |
| 7 | 2.330170  | -0.908254 | 0.750372  |
| 1 | 2.910596  | -0.104465 | 0.976681  |
| 1 | 2.147933  | -1.383705 | 1.630625  |
| 1 | 2.908155  | -1.545408 | 0.179457  |
| 7 | 0.027194  | 2.532662  | -1.400092 |
| 1 | 0.092688  | 3.142319  | -0.569583 |
| 1 | 0.814852  | 2.768889  | -1.998691 |
| 1 | -0.807350 | 2.817677  | -1.906889 |
| 7 | 4.033571  | -2.798316 | -0.940760 |
| 1 | 4.862372  | -3.066756 | -0.399829 |
| 1 | 4.370229  | -2.387243 | -1.807156 |
| 1 | 3.561386  | -3.660423 | -1.199127 |
| 7 | -6.768645 | -3.392905 | 0.697498  |
| 1 | -7.287710 | -2.610154 | 1.084245  |
| 1 | -6.549661 | -4.012306 | 1.472180  |
| 1 | -7.407235 | -3.897431 | 0.089439  |

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Cartesian coordinates of : BC10\_8

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.028215  | -0.041010 | 0.200188  |
| 1  | 1.651727  | -0.864605 | -0.041225 |
| 1  | 1.618882  | 0.810953  | -0.037912 |
| 1  | 0.115251  | -0.058411 | -0.354288 |
| 1  | 0.814673  | -0.048061 | 1.194922  |
| 7  | 5.589010  | 0.091059  | -1.342051 |
| 1  | 6.167321  | -0.462144 | -0.714587 |
| 1  | 5.684979  | -0.324591 | -2.265207 |
| 1  | 6.029802  | 1.006092  | -1.397723 |
| 7  | 2.905392  | 1.908660  | -0.553001 |
| 1  | 2.681818  | 2.417910  | -1.403995 |
| 1  | 3.713186  | 1.319239  | -0.762767 |
| 1  | 3.191411  | 2.604899  | 0.144453  |
| 7  | 3.010778  | -1.888403 | -0.572284 |
| 1  | 3.354257  | -2.564390 | 0.119073  |
| 1  | 2.819242  | -2.408167 | -1.424607 |
| 1  | 3.768617  | -1.237331 | -0.783095 |
| 7  | -3.718646 | -0.079404 | 0.773253  |
| 1  | -3.751588 | 0.700214  | 1.424379  |
| 1  | -4.560086 | -0.011224 | 0.185085  |
| 1  | -3.818696 | -0.921989 | 1.332695  |
| 7  | -6.237706 | 0.130007  | -1.025273 |
| 1  | -6.289268 | 1.014386  | -1.522819 |
| 1  | -7.092593 | 0.051040  | -0.466638 |
| 1  | -6.276424 | -0.599269 | -1.731638 |
| 7  | -1.411721 | -0.084816 | -1.193391 |
| 1  | -2.188714 | -0.084001 | -0.510799 |
| 1  | -1.552760 | 0.719508  | -1.799651 |
| 1  | -1.536317 | -0.906455 | -1.779688 |
| 7  | 3.701017  | 4.140558  | 1.517869  |
| 1  | 4.203206  | 3.822402  | 2.341685  |
| 1  | 2.871504  | 4.623954  | 1.850378  |
| 1  | 4.286368  | 4.841279  | 1.071974  |
| 7  | 3.983010  | -4.066781 | 1.477520  |
| 1  | 4.387640  | -3.724383 | 2.344204  |
| 1  | 4.676152  | -4.676396 | 1.052769  |
| 1  | 3.197100  | -4.656662 | 1.736035  |

|   |           |           |          |
|---|-----------|-----------|----------|
| 7 | -8.914277 | -0.107203 | 0.663399 |
| 1 | -9.727353 | 0.021352  | 0.068471 |
| 1 | -8.971533 | 0.590949  | 1.398682 |
| 1 | -9.013307 | -1.014769 | 1.108231 |

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Cartesian coordinates of : BTC10\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.011828  | -0.094443 | -0.667425 |
| 1  | 0.871680  | -0.536098 | -0.247974 |
| 1  | 0.045512  | -0.235830 | -1.675907 |
| 1  | -0.867829 | -0.550664 | -0.295156 |
| 1  | -0.001234 | 0.944952  | -0.488015 |
| 7  | 0.142765  | -3.363607 | 0.946019  |
| 1  | 0.165437  | -4.254224 | 0.438701  |
| 1  | 0.236661  | -3.587726 | 1.933086  |
| 1  | 0.971936  | -2.834091 | 0.686086  |
| 7  | -0.373746 | 2.721768  | -0.313498 |
| 1  | -0.109237 | 3.430470  | -0.993178 |
| 1  | -0.274242 | 3.146753  | 0.604768  |
| 1  | -1.374952 | 2.519487  | -0.458598 |
| 7  | -3.095346 | 1.515171  | -0.823892 |
| 1  | -3.835699 | 1.965028  | -0.274380 |
| 1  | -3.404619 | 1.528828  | -1.792074 |
| 1  | -3.054494 | 0.538786  | -0.540597 |
| 7  | 2.554536  | -1.030915 | 0.279252  |
| 1  | 2.776844  | -1.105635 | 1.268670  |
| 1  | 3.095938  | -1.747699 | -0.197294 |
| 1  | 2.899462  | -0.114760 | -0.045426 |
| 7  | -2.198121 | -1.580417 | 0.349562  |
| 1  | -1.533584 | -2.324749 | 0.618735  |
| 1  | -2.897745 | -2.003442 | -0.255262 |
| 1  | -2.681687 | -1.286428 | 1.194604  |
| 7  | 2.898455  | 1.786294  | -0.755057 |
| 1  | 3.656256  | 2.272544  | -0.263213 |
| 1  | 3.076136  | 1.904709  | -1.748861 |
| 1  | 2.032111  | 2.279012  | -0.549555 |
| 7  | 5.315922  | 3.235016  | 0.653208  |
| 1  | 6.168898  | 2.716335  | 0.464326  |
| 1  | 5.452696  | 4.168839  | 0.277010  |
| 1  | 5.250934  | 3.332790  | 1.662217  |
| 7  | 0.138979  | -6.195945 | -0.451066 |
| 1  | 0.948763  | -6.738959 | -0.165378 |
| 1  | 0.110898  | -6.224390 | -1.466045 |
| 1  | -0.680302 | -6.698871 | -0.122108 |
| 7  | -5.395430 | 2.995382  | 0.742861  |
| 1  | -5.333014 | 2.999670  | 1.756738  |
| 1  | -6.305464 | 2.609859  | 0.507309  |
| 1  | -5.404956 | 3.967372  | 0.447033  |

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Cartesian coordinates of : BL10\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.011932  | 1.700061  | -0.261812 |
| 1  | 0.031562  | 1.224841  | -1.162380 |
| 1  | -0.845033 | 1.354591  | 0.289615  |
| 1  | 0.920851  | 1.470640  | 0.266727  |
| 1  | -0.058484 | 2.726714  | -0.428913 |
| 7  | 2.383725  | 1.062661  | 1.056155  |
| 1  | 2.243731  | 0.493868  | 1.887819  |
| 1  | 2.986049  | 0.514570  | 0.416348  |
| 1  | 2.928887  | 1.868057  | 1.354181  |
| 7  | 8.919587  | -2.625768 | -0.687555 |
| 1  | 9.218882  | -2.193507 | -1.556458 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 9.750601  | -2.748294 | -0.116507 |
| 1 | 8.581119  | -3.554508 | -0.920514 |
| 7 | -0.191607 | 4.611962  | -0.748749 |
| 1 | -0.076250 | 5.149380  | 0.106661  |
| 1 | -1.094542 | 4.874881  | -1.135324 |
| 1 | 0.511545  | 4.951700  | -1.399911 |
| 7 | 4.171228  | -0.532992 | -0.776989 |
| 1 | 4.429391  | -0.092447 | -1.655795 |
| 1 | 3.839877  | -1.464444 | -1.012996 |
| 1 | 5.040483  | -0.654738 | -0.239291 |
| 7 | -6.506105 | -1.431804 | 0.996794  |
| 1 | -7.310744 | -1.729048 | 0.436685  |
| 1 | -6.188390 | -2.246917 | 1.513637  |
| 1 | -6.853678 | -0.772375 | 1.687249  |
| 7 | -2.227590 | 0.773682  | 1.116650  |
| 1 | -2.022543 | -0.004584 | 1.738861  |
| 1 | -2.686527 | 1.478247  | 1.689062  |
| 1 | -2.931574 | 0.434415  | 0.437148  |
| 7 | -9.022568 | -2.374700 | -0.687365 |
| 1 | -9.678797 | -2.872788 | -0.093281 |
| 1 | -9.529601 | -1.598541 | -1.102017 |
| 1 | -8.773027 | -3.003390 | -1.444907 |
| 7 | -4.301663 | -0.243810 | -0.825247 |
| 1 | -5.039974 | -0.638309 | -0.226233 |
| 1 | -4.001509 | -0.988408 | -1.448582 |
| 1 | -4.744730 | 0.456895  | -1.413265 |
| 7 | 6.771815  | -0.885983 | 0.867158  |
| 1 | 6.613629  | -1.355113 | 1.754473  |
| 1 | 7.226270  | -0.004009 | 1.086292  |
| 1 | 7.451253  | -1.450543 | 0.348345  |

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Cartesian coordinates of : L10

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Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | -1.189888  | 0.759104  | 0.354370  |
| 1  | -1.380670  | 1.272801  | 1.213346  |
| 1  | -0.272637  | 0.148579  | 0.482353  |
| 1  | -2.063711  | 0.136367  | 0.104984  |
| 1  | -1.035479  | 1.439593  | -0.388190 |
| 7  | -3.382784  | -0.743347 | -0.242083 |
| 1  | -3.450114  | -1.597835 | 0.306473  |
| 1  | -4.239332  | -0.188726 | -0.043371 |
| 1  | -3.435445  | -1.028641 | -1.217492 |
| 7  | -10.968990 | 0.350756  | -0.038158 |
| 1  | -11.098823 | 1.187294  | -0.599304 |
| 1  | -11.718089 | -0.289393 | -0.284853 |
| 1  | -11.116629 | 0.618835  | 0.930251  |
| 7  | 11.003811  | -0.658117 | -0.181880 |
| 1  | 11.815040  | -0.061177 | -0.312026 |
| 1  | 11.059383  | -1.391677 | -0.881902 |
| 1  | 11.105370  | -1.104420 | 0.724616  |
| 7  | -5.853626  | 0.826548  | 0.316861  |
| 1  | -5.959867  | 1.688475  | -0.211554 |
| 1  | -6.015478  | 1.069902  | 1.290510  |
| 1  | -6.628187  | 0.209032  | 0.033891  |
| 7  | 5.825441   | -0.755041 | 0.365680  |
| 1  | 6.645035   | -0.184878 | 0.120850  |
| 1  | 5.927808   | -1.014507 | 1.342807  |
| 1  | 5.895801   | -1.617373 | -0.167314 |
| 7  | 1.085731   | -0.683814 | 0.636125  |
| 1  | 1.295448   | -0.956722 | 1.593850  |
| 1  | 1.097973   | -1.541324 | 0.088259  |
| 1  | 1.883503   | -0.101634 | 0.306133  |
| 7  | 8.294607   | 0.990486  | -0.377082 |
| 1  | 9.163410   | 0.452101  | -0.315756 |
| 1  | 8.237251   | 1.358125  | -1.322389 |
| 1  | 8.397019   | 1.792503  | 0.238053  |
| 7  | 3.371652   | 0.958395  | -0.291080 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 4.193987  | 0.376973  | -0.067110 |
| 1 | 3.512260  | 1.851020  | 0.174759  |
| 1 | 3.415460  | 1.150756  | -1.288414 |
| 7 | -8.163570 | -1.033183 | -0.534866 |
| 1 | -8.184358 | -1.910126 | -0.021939 |
| 1 | -8.142331 | -1.278923 | -1.520637 |
| 1 | -9.060292 | -0.567502 | -0.364076 |

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Cartesian coordinates of the protonated ammonia undecamer

Cartesian coordinates of : BCa11\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.134826 | 0.454026  | -1.311986 |
| 1  | -0.403649 | 1.654227  | -1.575939 |
| 1  | -2.407734 | 0.458064  | -2.292428 |
| 1  | -2.107597 | -0.527333 | -1.027146 |
| 1  | -2.902876 | 0.887200  | -0.798212 |
| 7  | 0.654928  | -1.422604 | -1.687423 |
| 1  | 0.611217  | -1.711814 | -2.662004 |
| 1  | 0.573493  | -0.406541 | -1.685616 |
| 1  | -0.202434 | -1.768114 | -1.241942 |
| 7  | 2.349368  | 0.958751  | 0.130775  |
| 1  | 2.942367  | 0.169793  | -0.217269 |
| 1  | 2.924594  | 1.633075  | 0.672952  |
| 1  | 1.550678  | 0.577381  | 0.709824  |
| 7  | 0.490670  | 2.096909  | -1.822523 |
| 1  | 1.880680  | 1.431484  | -0.671115 |
| 1  | 0.602817  | 2.010421  | -2.829550 |
| 1  | 0.395363  | 3.091862  | -1.634810 |
| 7  | -1.782152 | -2.445483 | 0.069920  |
| 1  | -1.065493 | -2.844195 | 0.676120  |
| 1  | -2.325799 | -3.219987 | -0.301305 |
| 1  | -2.408481 | -1.892019 | 0.664127  |
| 7  | 1.247973  | -2.884704 | 1.103150  |
| 1  | 2.031857  | -2.597935 | 1.682554  |
| 1  | 1.405831  | -2.538531 | 0.156143  |
| 1  | 1.263372  | -3.900311 | 1.072867  |
| 7  | 3.723202  | -1.337876 | -0.991388 |
| 1  | 2.850734  | -1.694749 | -1.387245 |
| 1  | 4.131613  | -2.070425 | -0.417986 |
| 1  | 4.371330  | -1.171039 | -1.756054 |
| 7  | -0.013847 | -0.048177 | 1.338181  |
| 1  | -0.743314 | 0.108321  | 0.641420  |
| 1  | -0.361729 | 0.323753  | 2.217518  |
| 1  | 0.078889  | -1.060357 | 1.449844  |
| 7  | -3.671817 | -0.455588 | 1.604713  |
| 1  | -4.526791 | -0.994268 | 1.717431  |
| 1  | -3.926472 | 0.403510  | 1.115696  |
| 1  | -3.373278 | -0.197106 | 2.540860  |
| 7  | -4.739756 | 2.127319  | -0.076347 |
| 1  | -5.447849 | 1.767845  | -0.711650 |
| 1  | -4.335563 | 2.944744  | -0.526165 |
| 1  | -5.238228 | 2.472752  | 0.740180  |
| 7  | 4.060018  | 2.864418  | 1.659686  |
| 1  | 4.451432  | 3.589814  | 1.064463  |
| 1  | 4.848979  | 2.380938  | 2.081078  |
| 1  | 3.575702  | 3.340602  | 2.416072  |

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Cartesian coordinates of : BTC11\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

```

-----
7      0.514078      0.657074      -0.177165
1      0.355869      -0.336014      0.107972
1      1.540292      0.895586      -0.129337
1      0.150955      0.779892      -1.150230
1      -0.031937      1.269603      0.464998
7      -0.884941      0.829018      -2.702373
1      -0.719183      0.138182      -3.427709
1      -1.727882      0.562900      -2.183607
1      -1.056468      1.714505      -3.168499
7      -0.050651      -2.113182      0.611366
1      -1.018053      -2.312311      0.894583
1      0.159841      -2.729151      -0.169875
1      0.550102      -2.408201      1.376876
7      -1.105396      2.276922      1.697337
1      -0.622550      3.127503      1.974928
1      -1.293182      1.762713      2.554131
1      -2.011312      2.557158      1.312473
7      -2.771442      0.100674      -0.366443
1      -3.025390      0.971333      0.096777
1      -2.140782      -0.402486      0.255078
1      -3.607475      -0.477929      -0.437287
7      -3.016627      -2.615676      1.419875
1      -3.328638      -2.076489      2.223100
1      -3.695600      -2.454305      0.673686
1      -3.088634      -3.593899      1.686848
7      3.312218      1.307842      -0.073849
1      3.615575      1.768065      -0.928497
1      3.561676      1.933528      0.687852
1      3.895973      0.464933      0.031838
7      -3.957420      3.125978      0.504303
1      -4.072632      3.176150      -0.504699
1      -4.810743      2.718084      0.877326
1      -3.934821      4.086765      0.837158
7      5.128445      -1.156740      0.231680
1      4.963490      -1.891035      -0.451024
1      5.086616      -1.599376      1.145401
1      6.094232      -0.839482      0.099424
7      -5.151133      -2.144773      -1.014780
1      -4.737209      -2.234203      -1.939164
1      -5.906316      -1.469227      -1.098304
1      -5.594933      -3.036936      -0.811182
7      8.123821      -0.223825      -0.167412
1      8.759747      -0.986229      0.047684
1      8.380902      0.552807      0.434549
1      8.321809      0.064386      -1.121042
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Cartesian coordinates of : BDC11\_1

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Atomic number (AN) and Cartesian coordinates

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AN      X      Y      Z
-----
7      -0.955095      0.158895      -0.115460
1      -0.697798      -0.780789      0.292006
1      -1.290396      0.802000      0.635511
1      -0.068361      0.513426      -0.537717
1      -1.690338      0.053981      -0.849984
7      1.732441      0.565872      -1.144058
1      2.313694      1.394244      -1.012926
1      2.170599      -0.190376      -0.612875
1      1.812772      0.313186      -2.125722
7      0.157440      -2.286492      0.830977
1      0.012802      -2.567058      1.805609
1      -0.059191      -3.097885      0.258404
1      1.154226      -2.091465      0.705345
7      -3.036928      -0.089578      -2.173279
1      -3.952056      0.131523      -1.789551
1      -3.108725      -1.025789      -2.587381
1      -2.885708      0.559749      -2.940809
7      -1.896384      1.924259      2.040711

```

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.159725 | 2.541024  | 2.372938  |
| 1 | -2.695234 | 2.520366  | 1.797546  |
| 1 | -2.180618 | 1.365132  | 2.840884  |
| 7 | -3.379853 | -2.906292 | -3.526736 |
| 1 | -4.086192 | -2.821452 | -4.252215 |
| 1 | -2.541790 | -3.264833 | -3.974974 |
| 1 | -3.702491 | -3.626736 | -2.887374 |
| 7 | -4.349535 | 3.809545  | 1.452374  |
| 1 | -5.240806 | 3.322361  | 1.470754  |
| 1 | -4.309750 | 4.315786  | 0.572623  |
| 1 | -4.383965 | 4.507449  | 2.190082  |
| 7 | 3.346887  | -1.740587 | 0.547439  |
| 1 | 3.612071  | -2.650292 | 0.178525  |
| 1 | 3.490190  | -1.789315 | 1.553008  |
| 1 | 4.028300  | -1.063568 | 0.184499  |
| 7 | -0.306276 | -3.324773 | 3.803972  |
| 1 | -1.292394 | -3.446915 | 4.014754  |
| 1 | 0.083164  | -2.746616 | 4.542671  |
| 1 | 0.126944  | -4.239799 | 3.888510  |
| 7 | 3.528834  | 3.356208  | -1.003792 |
| 1 | 2.646166  | 3.827675  | -1.184043 |
| 1 | 4.167051  | 3.656224  | -1.736327 |
| 1 | 3.885910  | 3.739857  | -0.132610 |
| 7 | 5.136091  | 0.476109  | -0.715469 |
| 1 | 5.429200  | 0.201352  | -1.648600 |
| 1 | 5.980340  | 0.704273  | -0.198690 |
| 1 | 4.588753  | 1.331131  | -0.808621 |

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Cartesian coordinates of : BC11\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.783579 | 0.612200  | 0.277603  |
| 1  | -0.482491 | -0.014829 | 1.054574  |
| 1  | 0.068867  | 0.728444  | -0.309586 |
| 1  | -1.558145 | 0.163047  | -0.277466 |
| 1  | -1.099416 | 1.536400  | 0.657105  |
| 7  | -2.912244 | -0.622703 | -1.220384 |
| 1  | -2.591782 | -1.375327 | -1.824304 |
| 1  | -3.616288 | -1.029112 | -0.586497 |
| 1  | -3.402942 | 0.033454  | -1.822482 |
| 7  | 0.572920  | -1.132744 | 2.183613  |
| 1  | 0.652250  | -0.815228 | 3.145605  |
| 1  | 0.259419  | -2.098570 | 2.221577  |
| 1  | 1.516024  | -1.133587 | 1.783666  |
| 7  | -1.676022 | 3.162628  | 1.372771  |
| 1  | -1.851042 | 3.881321  | 0.660999  |
| 1  | -1.001960 | 3.554300  | 2.025440  |
| 1  | -2.541854 | 3.048695  | 1.893578  |
| 7  | -5.029957 | -1.849287 | 0.642763  |
| 1  | -5.499636 | -1.164534 | 1.228525  |
| 1  | -4.655352 | -2.553902 | 1.271852  |
| 1  | -5.754690 | -2.307247 | 0.081074  |
| 7  | -2.244462 | 5.445791  | -0.704854 |
| 1  | -3.085057 | 5.291977  | -1.254175 |
| 1  | -2.384339 | 6.312675  | -0.193570 |
| 1  | -1.490046 | 5.613195  | -1.364187 |
| 7  | 1.866604  | 0.549822  | -0.959122 |
| 1  | 1.948522  | 0.081011  | -1.857197 |
| 1  | 2.396576  | 1.413470  | -1.037556 |
| 1  | 2.357817  | -0.032643 | -0.276397 |
| 7  | 8.317131  | -1.472042 | -0.595393 |
| 1  | 8.975405  | -1.174364 | -1.309543 |
| 1  | 8.728446  | -1.232852 | 0.302030  |
| 1  | 8.274315  | -2.485927 | -0.638685 |
| 7  | 3.597571  | -1.266742 | 1.114951  |
| 1  | 4.261098  | -0.897856 | 0.419076  |
| 1  | 3.648675  | -2.280696 | 1.049771  |
| 1  | 3.978690  | -1.025198 | 2.026826  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -7.300658 | -3.282772 | -1.033432 |
| 1 | -6.940020 | -3.957921 | -1.701006 |
| 1 | -7.875610 | -2.629178 | -1.556763 |
| 1 | -7.922947 | -3.788360 | -0.409703 |
| 7 | 5.503868  | -0.104147 | -1.020493 |
| 1 | 5.234952  | -0.281556 | -1.984320 |
| 1 | 6.413424  | -0.556307 | -0.878969 |
| 1 | 5.660928  | 0.897168  | -0.945447 |

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Cartesian coordinates of : BC11\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.135560  | 0.293667  | -0.463278 |
| 1  | 0.404184  | 0.307534  | 0.541070  |
| 1  | -0.577486 | 1.041975  | -0.665233 |
| 1  | 1.020572  | 0.489975  | -0.973791 |
| 1  | -0.245521 | -0.649803 | -0.734342 |
| 7  | 2.871180  | 0.885159  | -1.362309 |
| 1  | 3.021992  | 1.727646  | -1.909976 |
| 1  | 3.336941  | 1.024449  | -0.462213 |
| 1  | 3.362304  | 0.135093  | -1.840606 |
| 7  | 1.487010  | 0.486222  | 2.134829  |
| 1  | 1.172860  | 1.201430  | 2.784480  |
| 1  | 1.584222  | -0.372079 | 2.669691  |
| 1  | 2.420232  | 0.753770  | 1.812729  |
| 7  | -0.934939 | -2.269949 | -1.234614 |
| 1  | -1.937926 | -2.215995 | -1.393253 |
| 1  | -0.786384 | -2.996857 | -0.519559 |
| 1  | -0.530871 | -2.621826 | -2.098812 |
| 7  | -1.823861 | 2.330389  | -1.033641 |
| 1  | -2.195785 | 2.252897  | -1.976861 |
| 1  | -2.627510 | 2.269643  | -0.391029 |
| 1  | -1.454410 | 3.274202  | -0.952387 |
| 7  | -0.540057 | -4.494211 | 0.859385  |
| 1  | -0.903307 | -5.369753 | 0.469570  |
| 1  | 0.427616  | -4.665538 | 1.117564  |
| 1  | -1.042894 | -4.325840 | 1.726180  |
| 7  | -4.238157 | 2.192410  | 0.866953  |
| 1  | -4.007533 | 2.455228  | 1.821057  |
| 1  | -4.670873 | 1.274615  | 0.920135  |
| 1  | -4.960053 | 2.844695  | 0.544844  |
| 7  | 4.521387  | 1.373649  | 1.389612  |
| 1  | 5.207730  | 1.653485  | 0.678944  |
| 1  | 4.945116  | 0.609481  | 1.910588  |
| 1  | 4.452773  | 2.153120  | 2.039813  |
| 7  | -1.645275 | -7.225513 | -0.297669 |
| 1  | -2.571696 | -7.140441 | -0.705155 |
| 1  | -1.711050 | -7.918251 | 0.442381  |
| 1  | -1.042578 | -7.617504 | -1.015144 |
| 7  | -6.491856 | 4.205764  | -0.076385 |
| 1  | -7.256966 | 4.214154  | 0.591752  |
| 1  | -6.891141 | 3.964885  | -0.978679 |
| 1  | -6.153578 | 5.160683  | -0.149205 |
| 7  | 6.599786  | 2.231065  | -0.805849 |
| 1  | 6.416383  | 3.149285  | -1.200214 |
| 1  | 6.699641  | 1.590012  | -1.587563 |
| 1  | 7.509547  | 2.285074  | -0.356007 |

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Cartesian coordinates of : BC11\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.437849  | -0.296487 | 0.099996  |
| 1  | 0.994926  | -1.051028 | -0.357051 |
| 1  | -0.512282 | -0.232546 | -0.331956 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.262321  | -0.531060 | 1.100622  |
| 1 | 0.951030  | 0.625467  | 0.023598  |
| 7 | -0.564680 | -0.894165 | 2.782990  |
| 1 | -1.555080 | -0.649670 | 2.666839  |
| 1 | -0.526846 | -1.862043 | 3.090050  |
| 1 | -0.205769 | -0.334419 | 3.551505  |
| 7 | 2.048202  | -2.381678 | -1.219539 |
| 1 | 2.960225  | -2.006662 | -1.466693 |
| 1 | 2.215507  | -3.218063 | -0.649494 |
| 1 | 1.624820  | -2.697734 | -2.087946 |
| 7 | 1.847303  | 2.187139  | -0.087852 |
| 1 | 2.572346  | 2.261693  | 0.632326  |
| 1 | 1.232017  | 2.986253  | 0.041445  |
| 1 | 2.302837  | 2.317245  | -0.996135 |
| 7 | -3.576561 | -0.025337 | 2.464926  |
| 1 | -3.797487 | 0.322684  | 3.394122  |
| 1 | -4.283359 | -0.723223 | 2.249241  |
| 1 | -3.710040 | 0.749175  | 1.812430  |
| 7 | 4.090294  | 2.544193  | 2.155209  |
| 1 | 4.765904  | 3.222760  | 1.816109  |
| 1 | 3.716516  | 2.912165  | 3.025004  |
| 1 | 4.609433  | 1.703424  | 2.389703  |
| 7 | -2.384834 | -0.301579 | -0.584516 |
| 1 | -2.769551 | -0.513886 | -1.509571 |
| 1 | -2.679694 | -1.043011 | 0.046824  |
| 1 | -2.837499 | 0.545817  | -0.244050 |
| 7 | 2.641192  | -5.004075 | 0.419869  |
| 1 | 3.276568  | -5.582395 | -0.122510 |
| 1 | 3.088377  | -4.839548 | 1.316956  |
| 1 | 1.815717  | -5.567432 | 0.601756  |
| 7 | -4.127704 | 2.413273  | 0.360224  |
| 1 | -4.875332 | 2.198030  | -0.294249 |
| 1 | -3.461731 | 2.997786  | -0.137953 |
| 1 | -4.538587 | 3.000389  | 1.081648  |
| 7 | -3.610837 | -1.022636 | -3.435857 |
| 1 | -4.617977 | -1.150431 | -3.400165 |
| 1 | -3.217220 | -1.897862 | -3.768975 |
| 1 | -3.427836 | -0.327611 | -4.153625 |
| 7 | 3.250839  | 2.755232  | -2.903712 |
| 1 | 3.347193  | 3.763146  | -2.986379 |
| 1 | 2.737280  | 2.440591  | -3.721410 |
| 1 | 4.185829  | 2.364843  | -2.974177 |

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Cartesian coordinates of : BC11\_4

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 2.363516  | 0.204679  | -0.453297 |
| 1  | 2.144538  | 0.118785  | 0.563228  |
| 1  | 2.855900  | -0.651124 | -0.805373 |
| 1  | 1.431306  | 0.305294  | -0.914444 |
| 1  | 2.948452  | 1.056043  | -0.633651 |
| 7  | -0.425450 | 0.486968  | -1.214771 |
| 1  | -0.861975 | -0.217879 | -1.802898 |
| 1  | -0.864883 | 0.403290  | -0.294881 |
| 1  | -0.709429 | 1.387082  | -1.592311 |
| 7  | 1.183116  | 0.047554  | 2.203853  |
| 1  | 1.302072  | -0.816157 | 2.725812  |
| 1  | 1.387037  | 0.805812  | 2.848989  |
| 1  | 0.190728  | 0.117895  | 1.955915  |
| 7  | 3.946638  | 2.585970  | -1.005631 |
| 1  | 4.173641  | 2.652902  | -1.994601 |
| 1  | 4.835760  | 2.634235  | -0.494461 |
| 1  | 3.432013  | 3.432434  | -0.776158 |
| 7  | 3.733741  | -2.136903 | -1.513093 |
| 1  | 4.628680  | -1.877950 | -1.920520 |
| 1  | 3.925001  | -2.876435 | -0.827311 |
| 1  | 3.195756  | -2.565282 | -2.262135 |
| 7  | 6.685636  | 2.881673  | 0.493617  |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | 7.035233   | 3.818313  | 0.311774  |
| 1 | 6.627846   | 2.782014  | 1.502904  |
| 1 | 7.402758   | 2.236044  | 0.175927  |
| 7 | 4.396626   | -4.492897 | 0.452637  |
| 1 | 3.579035   | -5.002612 | 0.774721  |
| 1 | 4.921673   | -4.226896 | 1.280582  |
| 1 | 4.972105   | -5.157106 | -0.057488 |
| 7 | -1.961269  | 0.230316  | 1.648665  |
| 1 | -2.654130  | 0.141354  | 0.890950  |
| 1 | -2.188914  | 1.088779  | 2.144916  |
| 1 | -2.155513  | -0.527409 | 2.299329  |
| 7 | -6.627875  | 0.252073  | 0.910031  |
| 1 | -7.451843  | 0.165898  | 0.307875  |
| 1 | -6.700749  | 1.146626  | 1.386282  |
| 1 | -6.708658  | -0.462572 | 1.627745  |
| 7 | -9.218773  | -0.006086 | -0.906092 |
| 1 | -9.302877  | 0.755360  | -1.572787 |
| 1 | -10.057628 | 0.007418  | -0.333624 |
| 1 | -9.237592  | -0.870147 | -1.439326 |
| 7 | -3.971392  | -0.010045 | -0.667830 |
| 1 | -3.996773  | -0.897557 | -1.162624 |
| 1 | -3.962833  | 0.714877  | -1.380140 |
| 1 | -4.867334  | 0.075576  | -0.168851 |

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Cartesian coordinates of : BC11\_5

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.005686  | 0.022909  | 0.070398  |
| 1  | -0.362585 | 0.926207  | 0.427678  |
| 1  | -0.410780 | -0.157238 | -0.863849 |
| 1  | 1.098849  | 0.045376  | 0.019266  |
| 1  | -0.314437 | -0.737037 | 0.700465  |
| 7  | 2.746292  | 0.072569  | -0.048290 |
| 1  | 3.092186  | 0.884684  | -0.567768 |
| 1  | 3.168076  | 0.108729  | 0.884366  |
| 1  | 3.117052  | -0.760626 | -0.514682 |
| 7  | -1.178852 | 2.561071  | 1.111591  |
| 1  | -1.354790 | 2.515509  | 2.111856  |
| 1  | -0.526602 | 3.327682  | 0.969153  |
| 1  | -2.060510 | 2.824209  | 0.664109  |
| 7  | -1.126428 | -2.240781 | 1.680314  |
| 1  | -0.353614 | -2.898316 | 1.751405  |
| 1  | -1.867238 | -2.706489 | 1.141718  |
| 1  | -1.473834 | -2.117222 | 2.627979  |
| 7  | 4.173059  | 0.169572  | 2.832723  |
| 1  | 4.438476  | -0.761684 | 3.139247  |
| 1  | 3.671371  | 0.601418  | 3.602831  |
| 1  | 5.033913  | 0.694898  | 2.710972  |
| 7  | 3.943655  | 2.555562  | -1.708500 |
| 1  | 3.988436  | 3.435150  | -1.202802 |
| 1  | 4.900474  | 2.293891  | -1.927378 |
| 1  | 3.481388  | 2.746075  | -2.592460 |
| 7  | -1.663395 | -0.596616 | -2.287807 |
| 1  | -1.750343 | 0.003828  | -3.102105 |
| 1  | -1.620090 | -1.552183 | -2.629084 |
| 1  | -2.509935 | -0.496809 | -1.723844 |
| 7  | 4.000134  | -2.486073 | -1.540714 |
| 1  | 3.799429  | -2.486356 | -2.536323 |
| 1  | 5.008363  | -2.408896 | -1.443839 |
| 1  | 3.740575  | -3.402038 | -1.187235 |
| 7  | -3.360902 | -0.049910 | 0.264025  |
| 1  | -4.242950 | -0.166604 | 0.756592  |
| 1  | -3.157955 | 0.949025  | 0.265730  |
| 1  | -2.645638 | -0.508788 | 0.827029  |
| 7  | -4.011649 | 3.128100  | -0.262222 |
| 1  | -4.341865 | 2.620830  | -1.079467 |
| 1  | -3.870827 | 4.089805  | -0.561504 |
| 1  | -4.783582 | 3.147991  | 0.399411  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -3.471381 | -3.189056 | -0.114584 |
| 1 | -3.742094 | -2.293167 | -0.515464 |
| 1 | -4.288096 | -3.574570 | 0.350991  |
| 1 | -3.254354 | -3.818712 | -0.881548 |

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Cartesian coordinates of : BL11\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.512599 | 0.014450  | 0.082168  |
| 1  | -0.124497 | 0.136132  | 1.036062  |
| 1  | -1.135164 | 0.832596  | -0.172186 |
| 1  | 0.318033  | -0.021742 | -0.537622 |
| 1  | -1.066514 | -0.885716 | 0.016927  |
| 7  | 2.191408  | -0.030010 | -1.138267 |
| 1  | 2.429868  | 0.718708  | -1.782236 |
| 1  | 2.774043  | 0.090938  | -0.306435 |
| 1  | 2.478767  | -0.898319 | -1.580653 |
| 7  | 1.178048  | 0.365361  | 2.487034  |
| 1  | 1.101419  | 1.249428  | 2.981577  |
| 1  | 1.165310  | -0.366576 | 3.191294  |
| 1  | 2.096638  | 0.343586  | 2.038688  |
| 7  | -2.082054 | -2.364214 | -0.111509 |
| 1  | -1.776255 | -3.133477 | 0.491711  |
| 1  | -2.122306 | -2.722082 | -1.070652 |
| 1  | -3.040866 | -2.155442 | 0.155865  |
| 7  | -2.263171 | 2.163268  | -0.606185 |
| 1  | -2.934437 | 2.343120  | 0.146769  |
| 1  | -1.802929 | 3.051791  | -0.824921 |
| 1  | -2.811523 | 1.915577  | -1.426091 |
| 7  | -2.362854 | -3.492075 | -3.085859 |
| 1  | -3.287286 | -3.903738 | -3.174626 |
| 1  | -2.277344 | -2.798672 | -3.822914 |
| 1  | -1.693155 | -4.227069 | -3.292895 |
| 7  | -1.011463 | 4.996573  | -1.392686 |
| 1  | -0.511078 | 5.001201  | -2.276438 |
| 1  | -0.397211 | 5.418676  | -0.702864 |
| 1  | -1.805431 | 5.620885  | -1.501384 |
| 7  | 4.231020  | 0.335101  | 1.366265  |
| 1  | 4.894086  | 0.263375  | 0.585765  |
| 1  | 4.486093  | -0.397478 | 2.024442  |
| 1  | 4.434598  | 1.215678  | 1.833212  |
| 7  | -1.336860 | -4.828631 | 1.781976  |
| 1  | -1.967565 | -5.579724 | 1.517297  |
| 1  | -1.494273 | -4.647040 | 2.768765  |
| 1  | -0.392814 | -5.192798 | 1.695465  |
| 7  | -4.434661 | 2.734818  | 1.663537  |
| 1  | -5.283980 | 3.071463  | 1.219417  |
| 1  | -4.131979 | 3.460561  | 2.306439  |
| 1  | -4.695766 | 1.931780  | 2.227736  |
| 7  | 6.258633  | 0.107786  | -1.028150 |
| 1  | 6.163285  | 0.833921  | -1.732150 |
| 1  | 6.226533  | -0.782021 | -1.517249 |
| 1  | 7.195558  | 0.195487  | -0.644394 |

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Cartesian coordinates of : BC11\_6

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.520680  | -0.027731 | -0.230683 |
| 1  | 1.041459  | -0.671091 | -0.863381 |
| 1  | -0.360576 | -0.491370 | 0.130611  |
| 1  | 1.128935  | 0.273125  | 0.559484  |
| 1  | 0.175246  | 0.803174  | -0.769162 |
| 7  | 2.201917  | 0.822429  | 2.051078  |
| 1  | 2.371603  | 0.051018  | 2.690858  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.118743  | 1.203827  | 1.794819  |
| 1 | 1.724577  | 1.540087  | 2.589946  |
| 7 | 1.948218  | -1.813442 | -2.108428 |
| 1 | 2.559367  | -1.285673 | -2.725945 |
| 1 | 2.523376  | -2.542870 | -1.673895 |
| 1 | 1.277772  | -2.286675 | -2.708419 |
| 7 | -0.908981 | 2.054460  | -1.633188 |
| 1 | -0.724229 | 3.041375  | -1.431511 |
| 1 | -1.864009 | 1.847650  | -1.333993 |
| 1 | -0.891706 | 1.955524  | -2.644713 |
| 7 | -2.879864 | -1.008230 | 3.620109  |
| 1 | -2.871291 | -0.127832 | 4.126237  |
| 1 | -2.248820 | -1.635708 | 4.109612  |
| 1 | -3.813763 | -1.395366 | 3.718218  |
| 7 | -0.327921 | 5.155511  | -1.184139 |
| 1 | -0.860258 | 5.700346  | -1.856191 |
| 1 | -0.559809 | 5.515840  | -0.263354 |
| 1 | 0.652321  | 5.366859  | -1.345418 |
| 7 | -2.069942 | -0.903833 | 0.505030  |
| 1 | -2.410148 | -1.778102 | 0.096466  |
| 1 | -2.314769 | -0.911141 | 1.498503  |
| 1 | -2.589416 | -0.142760 | 0.068307  |
| 7 | 3.746956  | -4.113582 | -0.914081 |
| 1 | 4.028726  | -4.728316 | -1.672326 |
| 1 | 4.600137  | -3.773739 | -0.480147 |
| 1 | 3.277478  | -4.693130 | -0.224602 |
| 7 | -4.063862 | 1.475789  | -0.834224 |
| 1 | -4.580437 | 0.704057  | -1.247582 |
| 1 | -4.325346 | 2.309461  | -1.354050 |
| 1 | -4.424649 | 1.597978  | 0.108194  |
| 7 | -3.187328 | -3.665173 | -0.718716 |
| 1 | -4.107240 | -3.863607 | -0.336561 |
| 1 | -2.581467 | -4.430774 | -0.438921 |
| 1 | -3.272230 | -3.710531 | -1.729705 |
| 7 | 5.042575  | 2.027457  | 1.391998  |
| 1 | 5.196526  | 2.865564  | 1.945205  |
| 1 | 5.178682  | 2.287298  | 0.419607  |
| 1 | 5.788074  | 1.379912  | 1.630509  |

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Cartesian coordinates of : P\_NH3\_N11\_18.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.718913  | 1.809199  | 0.376621  |
| 1  | 1.008467  | 2.731781  | 0.008322  |
| 1  | -0.294536 | 1.614258  | 0.211276  |
| 1  | 1.244921  | 1.007072  | -0.077751 |
| 1  | 0.856868  | 1.746397  | 1.409693  |
| 7  | 1.812008  | -0.555151 | -0.720630 |
| 1  | 0.967947  | -1.059982 | -0.996590 |
| 1  | 2.452826  | -0.549132 | -1.519646 |
| 1  | 2.247342  | -1.096937 | 0.025825  |
| 7  | 1.563488  | 4.526852  | -0.604109 |
| 1  | 2.574224  | 4.613247  | -0.667001 |
| 1  | 1.192800  | 4.767598  | -1.519245 |
| 1  | 1.249596  | 5.250596  | 0.036919  |
| 7  | 0.716090  | 1.086225  | 3.165195  |
| 1  | 0.373366  | 0.162640  | 2.880325  |
| 1  | 0.028886  | 1.506297  | 3.783957  |
| 1  | 1.560694  | 0.950975  | 3.712740  |
| 7  | 3.807337  | -0.552925 | -3.206970 |
| 1  | 4.698658  | -0.112952 | -2.997285 |
| 1  | 3.415309  | -0.054480 | -4.000613 |
| 1  | 4.014295  | -1.494581 | -3.527147 |
| 7  | -1.007692 | -2.208635 | -1.372368 |
| 1  | -0.926678 | -1.985801 | -2.361926 |
| 1  | -0.657015 | -3.158263 | -1.270470 |
| 1  | -2.014143 | -2.236201 | -1.165180 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -1.864069 | 0.580959  | 0.238214  |
| 1 | -1.623224 | -0.211105 | -0.358262 |
| 1 | -1.862198 | 0.214510  | 1.188318  |
| 1 | -2.822722 | 0.844298  | 0.009758  |
| 7 | 3.243227  | -2.387971 | 1.704493  |
| 1 | 3.502719  | -3.142966 | 1.074926  |
| 1 | 4.030819  | -1.745511 | 1.728809  |
| 1 | 3.182856  | -2.798685 | 2.632827  |
| 7 | -4.980340 | 1.316067  | -0.586188 |
| 1 | -5.834990 | 1.025085  | -0.118242 |
| 1 | -5.195485 | 1.364588  | -1.578779 |
| 1 | -4.804735 | 2.271861  | -0.286345 |
| 7 | -4.011840 | -1.868757 | -0.645249 |
| 1 | -4.235581 | -2.262541 | 0.264357  |
| 1 | -4.654546 | -2.289667 | -1.310264 |
| 1 | -4.224785 | -0.872275 | -0.600180 |
| 7 | 0.040908  | -1.616973 | 1.738723  |
| 1 | -0.445697 | -2.329858 | 2.276200  |
| 1 | 1.027457  | -1.882854 | 1.717459  |
| 1 | -0.299927 | -1.689650 | 0.779080  |

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Cartesian coordinates of : P\_NH3\_N11\_19.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.289684 | 1.841160  | -0.873099 |
| 1  | -0.119499 | 2.520324  | 0.711786  |
| 1  | -1.300528 | 2.667852  | -1.466583 |
| 1  | -1.041431 | 1.058271  | -1.480724 |
| 1  | -2.254216 | 1.685104  | -0.577263 |
| 7  | 1.887334  | 0.989135  | -1.443251 |
| 1  | 2.202462  | 1.644720  | -2.155102 |
| 1  | 1.444331  | 1.550767  | -0.716908 |
| 1  | 1.122491  | 0.449145  | -1.864318 |
| 7  | 2.048869  | 0.467498  | 1.985737  |
| 1  | 2.972519  | 0.400469  | 1.485419  |
| 1  | 2.175301  | 0.275393  | 2.976818  |
| 1  | 1.331798  | -0.222199 | 1.544769  |
| 7  | 0.570779  | 2.846564  | 1.402421  |
| 1  | 1.630277  | 1.424712  | 1.853138  |
| 1  | 1.026588  | 3.668927  | 1.015024  |
| 1  | 0.054982  | 3.167957  | 2.217879  |
| 7  | -0.455468 | -0.911548 | -2.420765 |
| 1  | 0.172154  | -1.692540 | -2.231513 |
| 1  | -0.681635 | -0.939784 | -3.411195 |
| 1  | -1.321748 | -1.088927 | -1.901094 |
| 7  | 2.311703  | -2.202414 | -1.277559 |
| 1  | 2.892622  | -2.638851 | -0.567250 |
| 1  | 2.551581  | -1.211665 | -1.322116 |
| 1  | 2.573444  | -2.625168 | -2.163934 |
| 7  | 4.392687  | 0.371001  | 0.348765  |
| 1  | 3.846718  | 0.538057  | -0.499853 |
| 1  | 4.933040  | -0.479322 | 0.217862  |
| 1  | 5.062439  | 1.128964  | 0.447460  |
| 7  | 0.175035  | -1.065100 | 0.703719  |
| 1  | -0.381438 | -0.394251 | 0.172076  |
| 1  | -0.493482 | -1.650244 | 1.210661  |
| 1  | 0.640219  | -1.656219 | 0.009265  |
| 7  | -2.919728 | -1.085727 | -0.478311 |
| 1  | -3.638298 | -1.650688 | -0.922750 |
| 1  | -3.357759 | -0.203800 | -0.211243 |
| 1  | -2.638857 | -1.571429 | 0.372091  |
| 7  | -4.502886 | 1.757675  | -0.044530 |
| 1  | -4.917100 | 1.894532  | -0.963189 |
| 1  | -4.371430 | 2.684127  | 0.353475  |
| 1  | -5.213078 | 1.305313  | 0.525732  |
| 7  | -1.999757 | -3.020548 | 2.140351  |
| 1  | -2.892452 | -2.794895 | 2.571830  |
| 1  | -1.387221 | -3.312123 | 2.897975  |

1      -2.154975      -3.846405      1.567434

Cartesian coordinates of :      P\_NH3\_N11\_10.log

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.000340 | -0.498728 | -0.000699 |
| 1  | -0.455984 | -1.086322 | -0.735480 |
| 1  | 0.770438  | 0.085559  | -0.394857 |
| 1  | -0.770173 | 0.087599  | 0.392256  |
| 1  | 0.454386  | -1.085590 | 0.735228  |
| 7  | -2.475035 | 0.839481  | 0.697921  |
| 1  | -2.559637 | 1.819927  | 0.443448  |
| 1  | -3.122502 | 0.321657  | 0.098328  |
| 1  | -2.831073 | 0.757584  | 1.646406  |
| 7  | -1.738040 | -1.861875 | -1.871066 |
| 1  | -2.638942 | -1.457727 | -1.596654 |
| 1  | -1.605611 | -1.663142 | -2.858859 |
| 1  | -1.821374 | -2.871241 | -1.787209 |
| 7  | 1.735507  | -1.860945 | 1.872101  |
| 1  | 1.603141  | -1.660678 | 2.859593  |
| 1  | 2.636879  | -1.458137 | 1.597266  |
| 1  | 1.817799  | -2.870515 | 1.789686  |
| 7  | -4.651885 | -0.743058 | -1.137351 |
| 1  | -5.033605 | -1.683621 | -1.067846 |
| 1  | -4.907156 | -0.404847 | -2.062254 |
| 1  | -5.178230 | -0.169366 | -0.463177 |
| 7  | -9.175345 | 0.974103  | 0.129246  |
| 1  | -9.535539 | 0.030039  | 0.025514  |
| 1  | -9.739577 | 1.427632  | 0.841945  |
| 1  | -9.361184 | 1.457590  | -0.744506 |
| 7  | 2.476395  | 0.833842  | -0.702666 |
| 1  | 2.832106  | 0.748450  | -1.650966 |
| 1  | 2.562613  | 1.814934  | -0.451251 |
| 1  | 3.123133  | 0.316872  | -0.101545 |
| 7  | 9.177449  | 0.975468  | -0.130010 |
| 1  | 9.711607  | 1.600145  | -0.727032 |
| 1  | 9.342075  | 1.271358  | 0.827620  |
| 1  | 9.589212  | 0.052038  | -0.227489 |
| 7  | 4.650654  | -0.745315 | 1.138532  |
| 1  | 5.178059  | -0.171473 | 0.465313  |
| 1  | 5.032567  | -1.685833 | 1.069451  |
| 1  | 4.904478  | -0.407281 | 2.063899  |
| 7  | -6.124674 | 1.012728  | 0.933219  |
| 1  | -5.841748 | 1.988377  | 0.963661  |
| 1  | -6.081245 | 0.670641  | 1.889346  |
| 1  | -7.113696 | 1.000386  | 0.661646  |
| 7  | 6.125386  | 1.012184  | -0.929210 |
| 1  | 6.080639  | 0.673083  | -1.886338 |
| 1  | 7.114747  | 0.998637  | -0.658939 |
| 1  | 5.842889  | 1.988060  | -0.956314 |

Cartesian coordinates of :      P\_NH3\_N11\_6.log

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.161793 | 0.158845  | -0.192242 |
| 1  | -1.126576 | -0.000812 | 0.838208  |
| 1  | -1.617328 | 1.076215  | -0.400555 |
| 1  | -0.151288 | 0.170810  | -0.493570 |
| 1  | -1.684182 | -0.611241 | -0.667505 |
| 7  | 1.672885  | 0.137668  | -0.473021 |
| 1  | 2.173350  | 0.980508  | -0.761190 |
| 1  | 1.873416  | 0.028002  | 0.523323  |
| 1  | 2.151505  | -0.638261 | -0.934105 |
| 7  | -0.516305 | -0.257072 | 2.626308  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.818139 | 0.461643  | 3.278434  |
| 1 | -0.784764 | -1.147648 | 3.035656  |
| 1 | 0.509522  | -0.232597 | 2.603710  |
| 7 | -2.659390 | -1.950965 | -1.579313 |
| 1 | -3.429291 | -1.545198 | -2.105078 |
| 1 | -3.066506 | -2.660993 | -0.960226 |
| 1 | -2.085287 | -2.446751 | -2.256151 |
| 7 | -2.425815 | 2.739374  | -0.792379 |
| 1 | -2.449235 | 2.924016  | -1.791917 |
| 1 | -3.392688 | 2.812976  | -0.455660 |
| 1 | -1.912331 | 3.510274  | -0.373124 |
| 7 | -3.981596 | -4.193027 | 0.186428  |
| 1 | -4.510305 | -4.800928 | -0.432795 |
| 1 | -3.319295 | -4.784133 | 0.680259  |
| 1 | -4.635609 | -3.842485 | 0.880192  |
| 7 | -5.381736 | 3.123563  | 0.199281  |
| 1 | -5.548288 | 2.827186  | 1.156516  |
| 1 | -6.072338 | 2.652555  | -0.377978 |
| 1 | -5.595980 | 4.116023  | 0.158759  |
| 7 | 2.657330  | -0.193522 | 2.748865  |
| 1 | 3.422687  | -0.138347 | 2.064883  |
| 1 | 2.812978  | -1.040947 | 3.289362  |
| 1 | 2.792002  | 0.579363  | 3.396198  |
| 7 | 3.595695  | 2.746366  | -1.285402 |
| 1 | 2.837057  | 3.225142  | -1.763529 |
| 1 | 4.341337  | 2.640839  | -1.968336 |
| 1 | 3.937892  | 3.389123  | -0.575957 |
| 7 | 3.540263  | -2.302196 | -1.791136 |
| 1 | 2.784239  | -2.637730 | -2.382025 |
| 1 | 3.817337  | -3.086425 | -1.206614 |
| 1 | 4.322176  | -2.109072 | -2.411486 |
| 7 | 4.655611  | 0.016844  | 0.387169  |
| 1 | 4.406827  | 0.888293  | -0.078486 |
| 1 | 4.386269  | -0.733342 | -0.247509 |
| 1 | 5.664782  | -0.007205 | 0.496376  |

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Cartesian coordinates of : P\_NH3\_N11\_4.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.498202 | 0.154749  | -0.102832 |
| 1  | -0.778207 | -0.261665 | -0.742192 |
| 1  | -1.760617 | -0.523896 | 0.649380  |
| 1  | -1.033439 | 0.994934  | 0.306637  |
| 1  | -2.348057 | 0.435467  | -0.645873 |
| 7  | 0.264529  | 2.321920  | 0.732445  |
| 1  | 0.296647  | 2.621859  | 1.702821  |
| 1  | 1.162818  | 1.868875  | 0.524331  |
| 1  | 0.209591  | 3.167462  | 0.171493  |
| 7  | 0.768872  | -0.531171 | -1.736015 |
| 1  | 1.378064  | -1.298076 | -1.432793 |
| 1  | 0.653352  | -0.616444 | -2.741996 |
| 1  | 1.304719  | 0.317466  | -1.558701 |
| 7  | -3.862462 | 0.916603  | -1.642621 |
| 1  | -3.616809 | 1.222397  | -2.580651 |
| 1  | -4.402724 | 1.677582  | -1.215141 |
| 1  | -4.499821 | 0.132912  | -1.757777 |
| 7  | -2.235695 | -1.737537 | 1.999514  |
| 1  | -2.898315 | -1.342367 | 2.661576  |
| 1  | -2.663763 | -2.591673 | 1.624160  |
| 1  | -1.428728 | -2.029475 | 2.544618  |
| 7  | -5.593996 | 3.240288  | -0.435489 |
| 1  | -5.115773 | 4.136510  | -0.428101 |
| 1  | -6.423711 | 3.356442  | -1.010400 |
| 1  | -5.916244 | 3.072183  | 0.513090  |
| 7  | -3.531548 | -4.397968 | 0.950443  |
| 1  | -3.133022 | -4.735815 | 0.079295  |
| 1  | -4.534895 | -4.328673 | 0.807125  |
| 1  | -3.385774 | -5.127792 | 1.642179  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 7 | 2.835866 | 0.587405  | 0.362446  |
| 1 | 3.367524 | 0.971510  | 1.149214  |
| 1 | 3.501927 | 0.386984  | -0.382942 |
| 1 | 2.474415 | -0.319343 | 0.650993  |
| 7 | 3.146341 | -2.396662 | -0.903626 |
| 1 | 3.190641 | -3.204439 | -1.518472 |
| 1 | 3.442289 | -2.717966 | 0.013688  |
| 1 | 3.840937 | -1.722156 | -1.230582 |
| 7 | 5.126493 | -0.075966 | -2.052806 |
| 1 | 4.783139 | 0.747671  | -2.539833 |
| 1 | 5.537055 | -0.676658 | -2.763150 |
| 1 | 5.893606 | 0.232455  | -1.461300 |
| 7 | 4.438155 | 1.906847  | 2.792642  |
| 1 | 3.973255 | 1.811022  | 3.690684  |
| 1 | 4.550469 | 2.902373  | 2.624591  |
| 1 | 5.370989 | 1.520782  | 2.905323  |

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Cartesian coordinates of : P\_NH3\_N11\_11.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.317543  | -0.039364 | -0.552567 |
| 1  | 0.956436  | -0.861683 | -0.456958 |
| 1  | -0.426973 | -0.038015 | 0.178721  |
| 1  | 0.941265  | 0.796539  | -0.476295 |
| 1  | -0.196352 | -0.054732 | -1.462191 |
| 7  | 2.468608  | 1.875974  | -0.311739 |
| 1  | 2.518125  | 2.428379  | 0.539835  |
| 1  | 3.261121  | 1.225606  | -0.292556 |
| 1  | 2.626664  | 2.518031  | -1.083541 |
| 7  | 2.502647  | -1.909594 | -0.266426 |
| 1  | 3.282667  | -1.244141 | -0.260656 |
| 1  | 2.561201  | -2.442123 | 0.597137  |
| 1  | 2.674045  | -2.565452 | -1.023645 |
| 7  | -1.571009 | -0.081170 | -2.750070 |
| 1  | -1.579677 | 0.719478  | -3.375871 |
| 1  | -2.450348 | -0.067044 | -2.224264 |
| 1  | -1.583516 | -0.909538 | -3.338625 |
| 7  | 5.049309  | 0.005958  | -0.306853 |
| 1  | 5.389657  | -0.020475 | -1.265358 |
| 1  | 5.463948  | -0.802872 | 0.166242  |
| 1  | 5.455556  | 0.845641  | 0.117317  |
| 7  | 6.269382  | -2.613970 | 1.051321  |
| 1  | 7.277287  | -2.533965 | 0.950317  |
| 1  | 6.082119  | -2.706574 | 2.045398  |
| 1  | 6.002079  | -3.492451 | 0.617091  |
| 7  | -2.131514 | -0.050544 | 1.007788  |
| 1  | -2.328830 | -0.872076 | 1.572799  |
| 1  | -2.340379 | 0.755177  | 1.591083  |
| 1  | -2.815360 | -0.046144 | 0.246656  |
| 7  | -8.901432 | 0.022679  | 0.973053  |
| 1  | -9.406746 | 0.013725  | 1.854266  |
| 1  | -9.230631 | 0.831015  | 0.453447  |
| 1  | -9.197221 | -0.799941 | 0.455826  |
| 7  | -4.430334 | -0.030422 | -1.298094 |
| 1  | -4.915759 | 0.014674  | -0.390824 |
| 1  | -4.787474 | -0.856985 | -1.771720 |
| 1  | -4.761272 | 0.766379  | -1.837313 |
| 7  | 6.245215  | 2.712446  | 0.893438  |
| 1  | 6.129389  | 2.813830  | 1.897508  |
| 1  | 5.904527  | 3.569851  | 0.468628  |
| 1  | 7.245215  | 2.677011  | 0.716819  |
| 7  | -5.786408 | 0.104571  | 1.473475  |
| 1  | -5.572519 | -0.667660 | 2.098576  |
| 1  | -6.797090 | 0.074048  | 1.301727  |
| 1  | -5.605200 | 0.956539  | 1.997148  |

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Cartesian coordinates of : P\_NH3\_N11\_5.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.341812  | -0.319398 | -0.257814 |
| 1  | 1.050235  | 0.486761  | 0.340038  |
| 1  | 1.741244  | -1.084596 | 0.333338  |
| 1  | 0.454395  | -0.635475 | -0.718972 |
| 1  | 2.041318  | -0.019600 | -0.975610 |
| 7  | -1.330494 | -0.732644 | -1.242104 |
| 1  | -1.797395 | -1.632012 | -1.365853 |
| 1  | -1.819672 | -0.247241 | -0.485439 |
| 1  | -1.511640 | -0.199669 | -2.089076 |
| 7  | -0.014279 | 1.760467  | 1.241823  |
| 1  | 0.184460  | 1.879384  | 2.231371  |
| 1  | -0.006129 | 2.690748  | 0.832880  |
| 1  | -0.976081 | 1.406241  | 1.167253  |
| 7  | 3.305981  | 0.441833  | -2.289257 |
| 1  | 4.187946  | -0.041183 | -2.138813 |
| 1  | 3.520912  | 1.444837  | -2.323812 |
| 1  | 2.993557  | 0.177358  | -3.220002 |
| 7  | 2.440790  | -2.474728 | 1.390411  |
| 1  | 2.739748  | -3.270817 | 0.833147  |
| 1  | 3.249017  | -2.189049 | 1.955063  |
| 1  | 1.741579  | -2.828256 | 2.038424  |
| 7  | 4.070653  | 3.480880  | -2.513248 |
| 1  | 4.888993  | 3.552549  | -3.111270 |
| 1  | 3.346023  | 4.050066  | -2.940928 |
| 1  | 4.311908  | 3.925450  | -1.632347 |
| 7  | 4.911439  | -1.731909 | 3.180993  |
| 1  | 4.851988  | -0.823483 | 3.631631  |
| 1  | 5.792966  | -1.751800 | 2.676456  |
| 1  | 4.984340  | -2.422639 | 3.922657  |
| 7  | -2.965012 | 0.684276  | 1.226551  |
| 1  | -3.626525 | 0.187020  | 0.621823  |
| 1  | -3.365272 | 1.606705  | 1.422061  |
| 1  | -2.962226 | 0.181848  | 2.111201  |
| 7  | -2.824459 | -3.616732 | -1.888322 |
| 1  | -1.932040 | -3.957846 | -2.236287 |
| 1  | -3.497981 | -3.770415 | -2.634443 |
| 1  | -3.089855 | -4.234441 | -1.125667 |
| 7  | -4.237726 | 3.536080  | 1.941505  |
| 1  | -4.313024 | 4.173737  | 1.154679  |
| 1  | -3.776368 | 4.043554  | 2.690523  |
| 1  | -5.184286 | 3.343772  | 2.256199  |
| 7  | -4.657829 | -1.060741 | -0.800010 |
| 1  | -4.059164 | -1.809495 | -1.145475 |
| 1  | -4.958225 | -0.517047 | -1.603717 |
| 1  | -5.490877 | -1.486655 | -0.404727 |

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Cartesian coordinates of : P\_NH3\_N11\_7.log-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.278998  | -0.310706 | 0.598234  |
| 1  | 1.290288  | 0.518722  | -0.059966 |
| 1  | 1.617949  | -0.036112 | 1.535694  |
| 1  | 0.265343  | -0.602199 | 0.637623  |
| 1  | 1.870672  | -1.084635 | 0.221512  |
| 7  | -1.526445 | -0.683392 | 0.337921  |
| 1  | -2.168973 | -0.530650 | 1.117292  |
| 1  | -1.662281 | 0.111544  | -0.291455 |
| 1  | -1.890482 | -1.494990 | -0.164577 |
| 7  | 0.893053  | 1.823745  | -1.232827 |
| 1  | 1.156948  | 2.775830  | -0.961886 |
| 1  | 1.296032  | 1.662344  | -2.152175 |
| 1  | -0.124637 | 1.802930  | -1.349719 |
| 7  | 2.924039  | -2.501498 | -0.469199 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 2.873569  | -3.335475 | 0.110133  |
| 1 | 3.918846  | -2.267829 | -0.564836 |
| 1 | 2.600416  | -2.777321 | -1.392762 |
| 7 | 2.320390  | 0.473637  | 3.332952  |
| 1 | 3.322710  | 0.639291  | 3.306518  |
| 1 | 1.892841  | 1.326643  | 3.682555  |
| 1 | 2.161697  | -0.243001 | 4.035775  |
| 7 | 5.991408  | -1.929307 | -0.853094 |
| 1 | 6.339320  | -2.581385 | -1.550425 |
| 1 | 6.214897  | -0.996609 | -1.187723 |
| 1 | 6.543000  | -2.079925 | -0.013366 |
| 7 | 1.740478  | 4.829570  | -0.600056 |
| 1 | 1.225643  | 5.285980  | 0.147095  |
| 1 | 1.557488  | 5.358910  | -1.447695 |
| 1 | 2.727614  | 4.944737  | -0.390379 |
| 7 | -2.302407 | 1.817932  | -1.728223 |
| 1 | -3.118532 | 1.246891  | -1.476502 |
| 1 | -2.264766 | 1.842560  | -2.744109 |
| 1 | -2.507063 | 2.768394  | -1.430460 |
| 7 | -3.896632 | -0.187247 | 2.646745  |
| 1 | -3.253094 | -0.308498 | 3.424142  |
| 1 | -4.628942 | -0.881244 | 2.771345  |
| 1 | -4.331169 | 0.723019  | 2.773440  |
| 7 | -2.991377 | -3.144250 | -1.394612 |
| 1 | -2.205399 | -3.775251 | -1.263017 |
| 1 | -3.100927 | -3.027067 | -2.398475 |
| 1 | -3.814540 | -3.642488 | -1.066550 |
| 7 | -4.430544 | -0.182768 | -0.683624 |
| 1 | -4.337693 | -0.124065 | 0.329205  |
| 1 | -4.053973 | -1.090370 | -0.952968 |
| 1 | -5.419528 | -0.168698 | -0.912798 |

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Cartesian coordinates of : P\_NH3\_N11\_23.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.000007  | -0.000045 | 0.326168  |
| 1  | -0.092507 | -0.846405 | 0.932627  |
| 1  | 0.852638  | -0.090185 | -0.279420 |
| 1  | -0.852618 | 0.090105  | -0.279428 |
| 1  | 0.092516  | 0.846304  | 0.932642  |
| 7  | -2.357011 | 0.235698  | -1.359194 |
| 1  | -2.340447 | -0.417966 | -2.137781 |
| 1  | -3.224505 | 0.051815  | -0.835379 |
| 1  | -2.452684 | 1.161215  | -1.768933 |
| 7  | -0.292474 | -2.338039 | 2.079434  |
| 1  | -1.238804 | -2.389214 | 2.447461  |
| 1  | -0.103415 | -3.237159 | 1.622759  |
| 1  | 0.324123  | -2.283317 | 2.885879  |
| 7  | 0.292473  | 2.337921  | 2.079481  |
| 1  | 0.103396  | 3.237047  | 1.622824  |
| 1  | 1.238805  | 2.389105  | 2.447502  |
| 1  | -0.324117 | 2.283173  | 2.885928  |
| 7  | -4.998017 | -0.297802 | 0.150809  |
| 1  | -5.159159 | 0.341111  | 0.924330  |
| 1  | -5.073943 | -1.235790 | 0.534034  |
| 1  | -5.779777 | -0.179709 | -0.501215 |
| 7  | 7.458888  | -0.034117 | -1.816736 |
| 1  | 8.325591  | 0.153643  | -1.321299 |
| 1  | 7.539139  | -0.968411 | -2.206881 |
| 1  | 7.422158  | 0.610305  | -2.600940 |
| 7  | 2.357045  | -0.235767 | -1.359173 |
| 1  | 2.452757  | -1.161303 | -1.768861 |
| 1  | 2.340458  | 0.417855  | -2.137794 |
| 1  | 3.224529  | -0.051822 | -0.835362 |
| 7  | 0.252194  | -5.168612 | 0.816598  |
| 1  | -0.089559 | -5.872413 | 1.464851  |
| 1  | -0.213125 | -5.336460 | -0.070565 |
| 1  | 1.239294  | -5.359665 | 0.671618  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 4.998017  | 0.297911  | 0.150816  |
| 1 | 5.779782  | 0.179859  | -0.501212 |
| 1 | 5.159202  | -0.340985 | 0.924342  |
| 1 | 5.073888  | 1.235908  | 0.534030  |
| 7 | -7.458873 | 0.034345  | -1.816742 |
| 1 | -7.422111 | -0.610009 | -2.601002 |
| 1 | -7.539148 | 0.968670  | -2.206808 |
| 1 | -8.325576 | -0.153485 | -1.321334 |
| 7 | -0.252249 | 5.168504  | 0.816702  |
| 1 | 0.089506  | 5.872296  | 1.464963  |
| 1 | -1.239353 | 5.359552  | 0.671738  |
| 1 | 0.213057  | 5.336370  | -0.070464 |

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Cartesian coordinates of : P\_NH3\_N11\_8.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.767686  | -0.137925 | 0.752692  |
| 1  | 1.287458  | 0.785032  | 0.535647  |
| 1  | 1.965654  | -0.211153 | 1.765456  |
| 1  | 1.072694  | -0.867345 | 0.459729  |
| 1  | 2.658706  | -0.231421 | 0.213968  |
| 7  | -0.467428 | -1.659808 | -0.212832 |
| 1  | -0.907593 | -2.450080 | 0.259724  |
| 1  | -1.140953 | -0.887913 | -0.194552 |
| 1  | -0.367891 | -1.931305 | -1.187724 |
| 7  | 0.159114  | 2.068801  | 0.059702  |
| 1  | 0.046150  | 2.842047  | 0.722069  |
| 1  | 0.372256  | 2.485823  | -0.842452 |
| 1  | -0.747494 | 1.599853  | -0.036418 |
| 7  | 4.314874  | -0.378761 | -0.680597 |
| 1  | 4.904771  | 0.428767  | -0.496465 |
| 1  | 4.226164  | -0.450890 | -1.700544 |
| 1  | 4.844432  | -1.191657 | -0.376291 |
| 7  | 2.388604  | -0.315939 | 3.708763  |
| 1  | 2.971497  | 0.462073  | 4.005097  |
| 1  | 1.545902  | -0.281779 | 4.275743  |
| 1  | 2.882189  | -1.165299 | 3.968996  |
| 7  | 4.233876  | -0.597599 | -3.814449 |
| 1  | 5.195468  | -0.569280 | -4.141602 |
| 1  | 3.831795  | -1.462682 | -4.163501 |
| 1  | 3.744462  | 0.162149  | -4.278215 |
| 7  | -0.173459 | 4.581112  | 1.992254  |
| 1  | -0.609278 | 4.395822  | 2.890750  |
| 1  | -0.761857 | 5.258236  | 1.515518  |
| 1  | 0.710429  | 5.043750  | 2.183183  |
| 7  | -2.719096 | 0.673422  | -0.128634 |
| 1  | -3.207866 | -0.225055 | -0.192399 |
| 1  | -3.047827 | 1.253603  | -0.905527 |
| 1  | -3.053400 | 1.117927  | 0.723023  |
| 7  | -1.717822 | -4.426045 | 1.133303  |
| 1  | -0.753542 | -4.709050 | 1.287585  |
| 1  | -2.157674 | -5.182927 | 0.616058  |
| 1  | -2.160918 | -4.403711 | 2.048031  |
| 7  | -3.863684 | 2.508773  | -2.506994 |
| 1  | -3.474525 | 3.442359  | -2.597006 |
| 1  | -4.854946 | 2.619062  | -2.314507 |
| 1  | -3.787682 | 2.067484  | -3.418486 |
| 7  | -3.836603 | -2.288524 | -0.267676 |
| 1  | -3.138851 | -2.909223 | 0.139973  |
| 1  | -3.975674 | -2.578162 | -1.231186 |
| 1  | -4.714498 | -2.447600 | 0.217582  |

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Cartesian coordinates of : P\_NH3\_N11\_17.log

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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7      0.396261      0.307951      0.783755
1      0.589547      0.816588      1.662121
1     -0.140813      0.914924      0.121645
1      1.325528     -0.024786      0.341586
1     -0.233410     -0.496565      0.970663
7      2.796351     -0.539859     -0.324780
1      3.472270      0.225643     -0.394192
1      3.230850     -1.275461      0.239139
1      2.674041     -0.917037     -1.268486
7      1.042498      1.774433      3.362769
1      0.906812      1.197804      4.188327
1      2.019553      2.053626      3.357296
1      0.495761      2.619394      3.502202
7     -1.779215     -1.687709      0.934208
1     -1.585959     -2.578325      0.484864
1     -2.497929     -1.217126      0.376238
1     -2.194751     -1.901604      1.836387
7      4.218949     -2.878440      1.387587
1      3.642224     -3.704012      1.518210
1      4.551101     -2.601505      2.306389
1      5.033647     -3.168614      0.854933
7      4.999649      1.801292     -0.654656
1      5.633331      1.900980      0.132619
1      5.560482      1.502134     -1.446950
1      4.650776      2.729370     -0.873950
7     -1.477299      1.562396     -1.029019
1     -1.833345      2.510073     -0.873869
1     -1.206641      1.505139     -2.006881
1     -2.252149      0.911290     -0.895004
7      2.526904     -1.738848     -3.312544
1      2.464530     -1.016679     -4.023782
1      3.379837     -2.259419     -3.494451
1      1.752624     -2.376827     -3.469176
7     -4.177078     -0.343881     -0.721171
1     -4.250623     -0.346991     -1.735552
1     -4.648950      0.499930     -0.405229
1     -4.740119     -1.134204     -0.386988
7     -2.562812      4.537319     -0.706331
1     -1.791089      5.195031     -0.767446
1     -3.059938      4.746819      0.154227
1     -3.194768      4.755692     -1.471163
7     -5.896531     -2.776591      0.309458
1     -6.712884     -2.875687     -0.287378
1     -6.241508     -2.646993      1.256173
1     -5.411774     -3.669057      0.292531
-----

```

Cartesian coordinates of : P\_NH3\_N11\_27.log

```

-----
Atomic number (AN) and Cartesian coordinates

```

```

AN      X      Y      Z
-----
7      2.338566     -0.495536      0.403997
1      2.472783     -0.671077      1.398607
1      1.434160      0.134048      0.254510
1      3.241173     -0.015774     -0.001520
1      2.196940     -1.394063     -0.055239
7      4.607379      0.668240     -0.565463
1      4.659627      1.667791     -0.381915
1      5.433269      0.233380     -0.108439
1      4.733654      0.558018     -1.569169
7     -12.293126     -0.601331     -0.220195
1     -13.106964     -0.007450     -0.093451
1     -12.304516     -0.922315     -1.183473
1     -12.425703     -1.418569      0.367692
7     -9.556241      0.884672      0.434777
1    -10.439283      0.409782      0.229619
1     -9.581633      1.783602     -0.037584
1     -9.544818      1.081640      1.431198
7      6.993770     -0.570447      0.726444

```

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 7.058004  | -1.583758 | 0.677573  |
| 1 | 7.139043  | -0.324375 | 1.702036  |
| 1 | 7.799663  | -0.197474 | 0.204348  |
| 7 | -4.549950 | 0.768199  | 0.547454  |
| 1 | -5.375876 | 0.247923  | 0.221526  |
| 1 | -4.640913 | 0.860623  | 1.555414  |
| 1 | -4.627001 | 1.707648  | 0.167642  |
| 7 | 0.102126  | 0.974675  | 0.020487  |
| 1 | -0.170053 | 1.552178  | 0.813067  |
| 1 | 0.154825  | 1.599282  | -0.781170 |
| 1 | -0.685914 | 0.316248  | -0.155928 |
| 7 | -7.050810 | -0.779435 | -0.423874 |
| 1 | -7.881927 | -0.244322 | -0.145833 |
| 1 | -7.097797 | -0.901402 | -1.431376 |
| 1 | -7.142575 | -1.706168 | -0.017805 |
| 7 | -2.162569 | -0.869156 | -0.431982 |
| 1 | -2.967237 | -0.316880 | -0.096054 |
| 1 | -2.183433 | -1.750543 | 0.074009  |
| 1 | -2.352884 | -1.097943 | -1.404188 |
| 7 | 9.398007  | 0.558624  | -0.845673 |
| 1 | 9.452432  | 1.572944  | -0.818499 |
| 1 | 9.398993  | 0.298130  | -1.827856 |
| 1 | 10.270508 | 0.202950  | -0.442816 |
| 7 | 12.129349 | -0.507974 | 0.353033  |
| 1 | 12.259005 | -0.257049 | 1.328583  |
| 1 | 12.911785 | -0.112689 | -0.160109 |
| 1 | 12.217163 | -1.518047 | 0.293570  |

-----

Cartesian coordinates of the protonated ammonia dodecamer

Cartesian coordinates of : BCa12\_1

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.864849  | -0.676755 | 1.802998  |
| 1  | 0.170369  | 0.366064  | 2.492530  |
| 1  | 2.029435  | -1.223904 | 2.645201  |
| 1  | 1.849389  | -1.343586 | 1.028514  |
| 1  | 2.693343  | -0.095481 | 1.670388  |
| 7  | -0.952578 | -2.276385 | 0.948662  |
| 1  | -1.006732 | -3.018571 | 1.642582  |
| 1  | -0.840375 | -1.406049 | 1.467417  |
| 1  | -0.068066 | -2.411071 | 0.445479  |
| 7  | -2.401581 | 0.858176  | 0.452498  |
| 1  | -3.042316 | 0.045456  | 0.310917  |
| 1  | -2.911796 | 1.748549  | 0.303561  |
| 1  | -1.558201 | 0.768203  | -0.193159 |
| 7  | -0.729257 | 0.711104  | 2.852253  |
| 1  | -1.996148 | 0.822891  | 1.412109  |
| 1  | -0.962218 | 0.152398  | 3.669327  |
| 1  | -0.573141 | 1.656513  | 3.192866  |
| 7  | 1.605412  | -2.409563 | -0.920810 |
| 1  | 0.935564  | -2.413019 | -1.689984 |
| 1  | 2.137582  | -3.273331 | -0.979986 |
| 1  | 2.256326  | -1.634581 | -1.090237 |
| 7  | -1.345812 | -2.134307 | -2.227069 |
| 1  | -2.072296 | -1.545400 | -2.624041 |
| 1  | -1.557024 | -2.280904 | -1.239445 |
| 1  | -1.405271 | -3.032868 | -2.697627 |
| 7  | -3.928071 | -1.610691 | 0.179138  |
| 1  | -3.099433 | -2.165742 | 0.405552  |
| 1  | -4.297676 | -1.944842 | -0.706198 |
| 1  | -4.636911 | -1.802126 | 0.881545  |
| 7  | -0.008693 | 0.404012  | -0.934505 |
| 1  | 0.621961  | 0.118069  | -0.183802 |
| 1  | 0.495273  | 1.102224  | -1.484435 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.127898 | -0.416739 | -1.532257 |
| 7 | 3.351463  | 0.188038  | -1.083154 |
| 1 | 4.166505  | 0.043472  | -1.672605 |
| 1 | 3.686599  | 0.557009  | -0.193237 |
| 1 | 2.778881  | 0.904038  | -1.527537 |
| 7 | 4.691924  | 1.061740  | 1.790819  |
| 1 | 5.341770  | 0.296850  | 1.954091  |
| 1 | 4.428018  | 1.418426  | 2.705629  |
| 1 | 5.225237  | 1.802212  | 1.342255  |
| 7 | 1.650206  | 2.392019  | -2.950700 |
| 1 | 2.409920  | 3.051138  | -2.802235 |
| 1 | 0.835899  | 2.948283  | -3.197870 |
| 1 | 1.890070  | 1.851986  | -3.778304 |
| 7 | -3.973131 | 3.385592  | 0.077681  |
| 1 | -3.416183 | 4.235792  | 0.069827  |
| 1 | -4.650725 | 3.490172  | 0.828409  |
| 1 | -4.502852 | 3.377609  | -0.789913 |

-----

Cartesian coordinates of : BCa12\_3

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.275179 | -0.658434 | -0.115396 |
| 1  | -1.012615 | -0.344034 | 0.554588  |
| 1  | 0.583481  | -0.917619 | 0.433758  |
| 1  | -0.654561 | -1.474829 | -0.662921 |
| 1  | -0.001630 | 0.122626  | -0.741189 |
| 7  | -1.579950 | -2.813735 | -1.471802 |
| 1  | -1.348791 | -3.752835 | -1.159382 |
| 1  | -2.557055 | -2.632422 | -1.202265 |
| 1  | -1.544452 | -2.831068 | -2.487352 |
| 7  | -2.372524 | 0.173323  | 1.744574  |
| 1  | -2.411123 | 1.187973  | 1.659442  |
| 1  | -3.212957 | -0.166399 | 1.278206  |
| 1  | -2.444610 | -0.074455 | 2.726991  |
| 7  | 0.982440  | 1.657812  | -1.464783 |
| 1  | 0.696971  | 2.271366  | -2.222694 |
| 1  | 1.951059  | 1.391317  | -1.641809 |
| 1  | 0.973946  | 2.201349  | -0.602414 |
| 7  | 2.143541  | -1.011416 | 1.404311  |
| 1  | 2.024749  | -1.003253 | 2.414436  |
| 1  | 2.708729  | -1.839122 | 1.186410  |
| 1  | 2.687585  | -0.180935 | 1.168131  |
| 7  | 4.052352  | 0.860572  | -2.472629 |
| 1  | 4.120440  | 1.629505  | -3.134851 |
| 1  | 5.007317  | 0.564424  | -2.285768 |
| 1  | 3.609971  | 0.089960  | -2.967278 |
| 7  | 3.809387  | -3.659327 | 0.985673  |
| 1  | 3.904226  | -4.025073 | 0.042775  |
| 1  | 3.343023  | -4.378868 | 1.530980  |
| 1  | 4.749086  | -3.573300 | 1.362374  |
| 7  | -4.461076 | -2.097864 | -0.622171 |
| 1  | -5.092945 | -2.347910 | -1.378114 |
| 1  | -4.581547 | -1.096473 | -0.448758 |
| 1  | -4.797238 | -2.590508 | 0.200767  |
| 7  | -4.736630 | 1.054586  | -0.118342 |
| 1  | -3.902966 | 1.647100  | -0.106580 |
| 1  | -5.332392 | 1.359005  | 0.647374  |
| 1  | -5.244777 | 1.269813  | -0.972313 |
| 7  | 3.589865  | 1.850451  | 0.592849  |
| 1  | 3.774119  | 1.526200  | -0.359146 |
| 1  | 4.425068  | 1.663428  | 1.142359  |
| 1  | 3.512696  | 2.863858  | 0.541636  |
| 7  | -1.918680 | 2.659816  | -0.144610 |
| 1  | -1.055520 | 2.551548  | 0.395174  |
| 1  | -2.123004 | 3.653819  | -0.201249 |
| 1  | -1.712962 | 2.345591  | -1.089751 |
| 7  | 0.576926  | 1.916065  | 1.723593  |
| 1  | 1.566134  | 1.743865  | 1.527727  |

```

1      0.181292      1.043856      2.068577
1      0.537949      2.579555      2.493251
-----

```

Cartesian coordinates of : BC12\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | 2.734362   | -0.128703 | -0.265332 |
| 1  | 2.491801   | 0.171802  | 0.706206  |
| 1  | 2.597339   | -1.160676 | -0.372335 |
| 1  | 2.068862   | 0.394940  | -0.881606 |
| 1  | 3.722413   | 0.126221  | -0.498539 |
| 7  | 0.748886   | 1.556170  | -1.516505 |
| 1  | -0.179520  | 1.120962  | -1.539816 |
| 1  | 0.699922   | 2.287001  | -0.810101 |
| 1  | 0.895271   | 2.013177  | -2.412115 |
| 7  | 1.651274   | 0.955763  | 2.200502  |
| 1  | 1.425915   | 0.304396  | 2.947381  |
| 1  | 2.158183   | 1.723217  | 2.632642  |
| 1  | 0.763137   | 1.334525  | 1.849571  |
| 7  | 5.489340   | 0.535325  | -0.981160 |
| 1  | 6.126970   | -0.216576 | -0.732632 |
| 1  | 5.855533   | 1.389328  | -0.545244 |
| 1  | 5.575895   | 0.659710  | -1.986627 |
| 7  | 2.336395   | -3.007791 | -0.586713 |
| 1  | 2.362021   | -3.278927 | -1.566293 |
| 1  | 3.035914   | -3.581438 | -0.101880 |
| 1  | 1.426639   | -3.295482 | -0.235664 |
| 7  | 6.754769   | 3.123627  | 0.271070  |
| 1  | 7.676591   | 3.243177  | -0.139322 |
| 1  | 6.238557   | 3.978264  | 0.084004  |
| 1  | 6.886977   | 3.074478  | 1.277081  |
| 7  | 4.409673   | -4.873468 | 0.859636  |
| 1  | 3.984778   | -5.788375 | 0.981440  |
| 1  | 4.696992   | -4.558951 | 1.781813  |
| 1  | 5.258674   | -5.016284 | 0.320287  |
| 7  | -1.117454  | 1.971880  | 1.105704  |
| 1  | -1.451617  | 1.457987  | 0.288703  |
| 1  | -1.285060  | 2.957902  | 0.921852  |
| 1  | -1.742852  | 1.720639  | 1.867191  |
| 7  | -4.342875  | 0.433644  | 0.651570  |
| 1  | -5.172256  | 0.101764  | 0.141225  |
| 1  | -4.557781  | 1.371972  | 0.978108  |
| 1  | -4.257274  | -0.148073 | 1.480571  |
| 7  | -6.809304  | -0.552229 | -0.955515 |
| 1  | -6.938678  | -0.012789 | -1.806717 |
| 1  | -7.677767  | -0.476691 | -0.418065 |
| 1  | -6.719291  | -1.522981 | -1.241406 |
| 7  | -2.175004  | 0.317620  | -1.539372 |
| 1  | -2.007341  | -0.647513 | -1.811730 |
| 1  | -2.578687  | 0.774957  | -2.353211 |
| 1  | -2.912617  | 0.298371  | -0.821431 |
| 7  | -9.525042  | -0.320596 | 0.674059  |
| 1  | -9.582704  | -0.998461 | 1.428046  |
| 1  | -10.327479 | -0.478012 | 0.071732  |
| 1  | -9.642597  | 0.597752  | 1.091285  |

-----  
Cartesian coordinates of : BC12\_4

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.599682 | -0.167814 | -0.411924 |
| 1  | -0.318510 | -0.131625 | 0.589827  |
| 1  | -1.214192 | 0.650120  | -0.656265 |
| 1  | 0.297787  | -0.119740 | -0.937687 |
| 1  | -1.100145 | -1.069024 | -0.622110 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 2.172170  | -0.006626 | -1.344971 |
| 1 | 2.455460  | 0.878238  | -1.756893 |
| 1 | 2.660102  | -0.087995 | -0.449690 |
| 1 | 2.544601  | -0.736715 | -1.945817 |
| 7 | 0.768174  | -0.061878 | 2.173805  |
| 1 | 0.674616  | 0.800522  | 2.702775  |
| 1 | 0.614359  | -0.823370 | 2.828655  |
| 1 | 1.740244  | -0.122860 | 1.857032  |
| 7 | -1.986547 | -2.631824 | -1.004865 |
| 1 | -2.327345 | -2.659683 | -1.962457 |
| 1 | -2.805952 | -2.758485 | -0.392997 |
| 1 | -1.402631 | -3.455949 | -0.888201 |
| 7 | -2.308640 | 2.053660  | -1.114593 |
| 1 | -3.287900 | 1.779853  | -1.115273 |
| 1 | -2.222553 | 2.848339  | -0.464725 |
| 1 | -2.114851 | 2.413360  | -2.045669 |
| 7 | -4.438687 | -3.050272 | 0.810535  |
| 1 | -4.944462 | -3.890550 | 0.513410  |
| 1 | -4.190364 | -3.184195 | 1.786704  |
| 1 | -5.102678 | -2.281515 | 0.787277  |
| 7 | -2.107780 | 4.467661  | 0.792304  |
| 1 | -1.169642 | 4.845260  | 0.890677  |
| 1 | -2.437153 | 4.267772  | 1.732534  |
| 1 | -2.695630 | 5.222298  | 0.424569  |
| 7 | 3.882603  | -0.313442 | 1.408741  |
| 1 | 4.537770  | -0.470455 | 0.630102  |
| 1 | 3.999896  | -1.100512 | 2.042566  |
| 1 | 4.221891  | 0.503823  | 1.910436  |
| 7 | -6.032425 | -5.643106 | -0.065149 |
| 1 | -6.452429 | -5.555509 | -0.985737 |
| 1 | -6.788089 | -5.830771 | 0.587207  |
| 1 | -5.447378 | -6.473077 | -0.085702 |
| 7 | -3.907854 | 6.830397  | -0.305597 |
| 1 | -3.940997 | 7.590938  | 0.366939  |
| 1 | -4.867821 | 6.547534  | -0.478732 |
| 1 | -3.553939 | 7.220054  | -1.174225 |
| 7 | 5.746094  | -0.768205 | -1.015994 |
| 1 | 5.682952  | -0.057729 | -1.739903 |
| 1 | 5.622551  | -1.664053 | -1.479889 |
| 1 | 6.709575  | -0.748982 | -0.665401 |
| 7 | 8.722910  | -0.730612 | 0.038036  |
| 1 | 9.373724  | -0.943121 | -0.712426 |
| 1 | 8.880724  | -1.418512 | 0.768488  |
| 1 | 8.996053  | 0.170742  | 0.418308  |

-----

Cartesian coordinates of : BC12\_2

-----

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.150444 | 0.944434  | 0.280429  |
| 1  | -0.333714 | 0.251760  | 1.037712  |
| 1  | 0.688375  | 0.651438  | -0.289445 |
| 1  | -1.012724 | 0.930006  | -0.302443 |
| 1  | 0.005017  | 1.896655  | 0.687453  |
| 7  | -2.757989 | 0.452652  | -0.962480 |
| 1  | -2.755054 | 0.001940  | -1.873438 |
| 1  | -3.135672 | -0.226807 | -0.297630 |
| 1  | -3.433563 | 1.209758  | -1.018824 |
| 7  | -1.167258 | -1.076866 | 2.126931  |
| 1  | -2.095113 | -1.238285 | 1.724206  |
| 1  | -0.678433 | -1.967674 | 2.130142  |
| 1  | -1.300403 | -0.814702 | 3.099525  |
| 7  | 0.314117  | 3.577875  | 1.450875  |
| 1  | 0.336743  | 4.339070  | 0.762717  |
| 1  | 1.205718  | 3.596941  | 1.939252  |
| 1  | -0.392143 | 3.824914  | 2.139210  |
| 7  | -4.121644 | -1.723864 | 1.043344  |
| 1  | -4.510798 | -1.646920 | 1.980201  |
| 1  | -3.993741 | -2.718745 | 0.873876  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -4.861004 | -1.411562 | 0.398243  |
| 7 | 0.411530  | 5.989323  | -0.558492 |
| 1 | -0.496179 | 6.231297  | -0.945069 |
| 1 | 0.744077  | 6.808616  | -0.057914 |
| 1 | 1.038579  | 5.852536  | -1.345850 |
| 7 | 2.145634  | 0.139533  | -1.239201 |
| 1 | 1.948617  | -0.593549 | -1.915778 |
| 1 | 2.568215  | 0.901130  | -1.763940 |
| 1 | 2.876242  | -0.226920 | -0.608796 |
| 7 | 9.285449  | -2.667279 | 0.179177  |
| 1 | 10.082250 | -2.763736 | -0.443108 |
| 1 | 9.593630  | -2.113431 | 0.972620  |
| 1 | 9.069686  | -3.595094 | 0.531111  |
| 7 | 4.360754  | -0.953510 | 0.560367  |
| 1 | 5.179264  | -1.081201 | -0.048458 |
| 1 | 4.161200  | -1.857273 | 0.979919  |
| 1 | 4.649061  | -0.343999 | 1.320549  |
| 7 | -6.264482 | -0.711815 | -0.940527 |
| 1 | -5.999926 | -0.751922 | -1.920898 |
| 1 | -6.579949 | 0.238431  | -0.766071 |
| 1 | -7.083148 | -1.319284 | -0.829366 |
| 7 | 6.814830  | -1.341609 | -1.314902 |
| 1 | 6.592518  | -1.943301 | -2.102778 |
| 1 | 7.603573  | -1.770680 | -0.822622 |
| 1 | 7.149656  | -0.466286 | -1.707141 |
| 7 | -8.799728 | -2.563092 | -0.600988 |
| 1 | -8.592038 | -3.545875 | -0.751544 |
| 1 | -9.527091 | -2.310767 | -1.263700 |
| 1 | -9.207115 | -2.486967 | 0.326351  |

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Cartesian coordinates of : BL12\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.093298 | -0.459045 | -0.238434 |
| 1  | -0.131415 | -1.191474 | -0.981603 |
| 1  | -0.953965 | -0.517532 | 0.357604  |
| 1  | 0.755769  | -0.605500 | 0.359211  |
| 1  | -0.044831 | 0.487239  | -0.688472 |
| 7  | 2.257239  | -0.837083 | 1.440660  |
| 1  | 2.188912  | -1.647929 | 2.049984  |
| 1  | 3.117059  | -0.952223 | 0.886015  |
| 1  | 2.405484  | -0.036439 | 2.049466  |
| 7  | -0.207607 | -2.475042 | -2.381491 |
| 1  | 0.605020  | -2.414949 | -2.989238 |
| 1  | -0.257655 | -3.443387 | -2.046786 |
| 1  | -1.019338 | -2.326302 | -2.975108 |
| 7  | 0.032379  | 2.163058  | -1.498556 |
| 1  | 0.250982  | 2.904974  | -0.818828 |
| 1  | -0.846821 | 2.419125  | -1.940192 |
| 1  | 0.740814  | 2.212969  | -2.226002 |
| 7  | 4.871239  | -1.170471 | -0.174929 |
| 1  | 5.095004  | -0.349648 | -0.730454 |
| 1  | 4.859890  | -1.957129 | -0.817847 |
| 1  | 5.656020  | -1.320276 | 0.466522  |
| 7  | 0.681332  | 4.432119  | 0.496396  |
| 1  | 1.596003  | 4.341580  | 0.929432  |
| 1  | 0.673265  | 5.329125  | 0.001278  |
| 1  | 0.010474  | 4.506549  | 1.255851  |
| 7  | -2.478294 | -0.600940 | 1.430454  |
| 1  | -2.507764 | -1.436511 | 2.008779  |
| 1  | -2.535783 | 0.188038  | 2.069087  |
| 1  | -3.343182 | -0.594513 | 0.871811  |
| 7  | -0.368929 | -5.487538 | -1.477249 |
| 1  | -0.347247 | -6.079260 | -2.302842 |
| 1  | 0.403016  | -5.780133 | -0.885511 |
| 1  | -1.224205 | -5.712003 | -0.977398 |
| 7  | -5.111037 | -0.569891 | -0.189756 |
| 1  | -5.904555 | -0.582590 | 0.458376  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -5.222605 | -1.367110 | -0.809681 |
| 1 | -5.214432 | 0.259131  | -0.768060 |
| 7 | 7.331330  | -1.635284 | 1.770242  |
| 1 | 7.281334  | -2.524966 | 2.257594  |
| 1 | 7.409932  | -0.913817 | 2.480738  |
| 1 | 8.203194  | -1.632940 | 1.249091  |
| 7 | -7.598115 | -0.607218 | 1.775174  |
| 1 | -7.614485 | -1.428825 | 2.372015  |
| 1 | -8.467071 | -0.606989 | 1.249178  |
| 1 | -7.623475 | 0.202748  | 2.387415  |
| 7 | 0.678278  | 7.228609  | -0.995588 |
| 1 | 0.920938  | 7.976202  | -0.352167 |
| 1 | -0.226972 | 7.462731  | -1.392085 |
| 1 | 1.351077  | 7.263121  | -1.755644 |

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Cartesian coordinates of : BC12\_3

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.605941  | -0.060948 | 0.011097  |
| 1  | -0.105974 | -0.782931 | 0.308566  |
| 1  | 1.181027  | -0.417176 | -0.777730 |
| 1  | 0.025086  | 0.769529  | -0.300007 |
| 1  | 1.216252  | 0.198014  | 0.811216  |
| 7  | -1.298153 | 1.904102  | -0.726951 |
| 1  | -1.335816 | 2.160469  | -1.716421 |
| 1  | -2.154212 | 1.391536  | -0.511189 |
| 1  | -1.317240 | 2.771466  | -0.185300 |
| 7  | -1.647777 | -1.656332 | 0.694432  |
| 1  | -1.829916 | -2.498671 | 0.143731  |
| 1  | -1.781087 | -1.897940 | 1.679252  |
| 1  | -2.362226 | -0.970943 | 0.448132  |
| 7  | 2.297264  | 0.659187  | 2.356376  |
| 1  | 2.638750  | -0.170104 | 2.834486  |
| 1  | 1.734435  | 1.168127  | 3.032584  |
| 1  | 3.114610  | 1.242296  | 2.149676  |
| 7  | 2.203785  | -1.043393 | -2.303436 |
| 1  | 1.579207  | -1.434733 | -3.003290 |
| 1  | 2.698800  | -0.280025 | -2.756372 |
| 1  | 2.899717  | -1.764490 | -2.087832 |
| 7  | -1.382451 | 4.696660  | 0.899789  |
| 1  | -1.596857 | 4.625058  | 1.889712  |
| 1  | -0.493499 | 5.181388  | 0.822743  |
| 1  | -2.086083 | 5.301812  | 0.487395  |
| 7  | -1.430537 | 2.804634  | -3.829448 |
| 1  | -0.553080 | 3.220483  | -4.126663 |
| 1  | -2.146763 | 3.516293  | -3.938799 |
| 1  | -1.646554 | 2.063855  | -4.489494 |
| 7  | -4.214954 | 0.386005  | -0.012422 |
| 1  | -4.616362 | 1.239838  | -0.390543 |
| 1  | -4.537232 | 0.312956  | 0.948601  |
| 1  | -4.636212 | -0.384962 | -0.523265 |
| 7  | -2.080959 | -2.513196 | 3.780544  |
| 1  | -1.312007 | -3.109854 | 4.070451  |
| 1  | -2.930888 | -3.061364 | 3.873190  |
| 1  | -2.140864 | -1.758093 | 4.456827  |
| 7  | 4.373130  | -3.275073 | -1.751751 |
| 1  | 5.271887  | -2.882703 | -1.487195 |
| 1  | 4.528826  | -3.822773 | -2.593044 |
| 1  | 4.109419  | -3.927231 | -1.019176 |
| 7  | -2.253924 | -4.360432 | -0.967515 |
| 1  | -1.460211 | -4.989718 | -0.895120 |
| 1  | -2.451098 | -4.244943 | -1.956908 |
| 1  | -3.050525 | -4.841837 | -0.561198 |
| 7  | 4.842094  | 2.463629  | 1.844284  |
| 1  | 4.736764  | 3.116015  | 1.073064  |
| 1  | 5.672813  | 1.911716  | 1.651851  |
| 1  | 5.042893  | 3.015736  | 2.673066  |

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Cartesian coordinates of : P\_NH3\_N12\_32.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.017628 | -0.055677 | -0.033721 |
| 1  | -0.154789 | 0.400240  | -0.449682 |
| 1  | -1.174226 | 0.349418  | 0.908842  |
| 1  | -1.850783 | 0.128978  | -0.638376 |
| 1  | -0.859792 | -1.087378 | 0.039179  |
| 7  | 1.876334  | -4.099295 | -1.616507 |
| 1  | 2.375516  | -4.784214 | -1.054689 |
| 1  | 2.561198  | -3.680184 | -2.240233 |
| 1  | 1.238151  | -4.623784 | -2.209495 |
| 7  | 2.398673  | -1.575916 | 0.528974  |
| 1  | 3.324769  | -1.851830 | 0.845455  |
| 1  | 1.747899  | -1.779048 | 1.289893  |
| 1  | 2.154071  | -2.204303 | -0.236146 |
| 7  | 1.396034  | 1.068298  | -1.023805 |
| 1  | 2.026839  | 0.323675  | -0.722231 |
| 1  | 1.525718  | 1.221423  | -2.027415 |
| 1  | 1.675033  | 1.921343  | -0.541205 |
| 7  | -3.341699 | 0.442558  | -1.750872 |
| 1  | -3.281900 | 1.344346  | -2.216385 |
| 1  | -4.238423 | 0.424546  | -1.251995 |
| 1  | -3.402282 | -0.254778 | -2.488215 |
| 7  | 0.310127  | -1.469050 | 3.001542  |
| 1  | 0.699076  | -0.527689 | 2.925382  |
| 1  | -0.695494 | -1.358476 | 3.104857  |
| 1  | 0.652426  | -1.873610 | 3.868778  |
| 7  | -1.139840 | 1.413740  | 2.550403  |
| 1  | -1.509854 | 2.340826  | 2.359087  |
| 1  | -0.120811 | 1.494104  | 2.620290  |
| 1  | -1.494876 | 1.147095  | 3.464350  |
| 7  | -0.513673 | -2.916900 | 0.270409  |
| 1  | -1.295023 | -3.565024 | 0.238306  |
| 1  | -0.159036 | -2.900672 | 1.226836  |
| 1  | 0.220384  | -3.289233 | -0.334128 |
| 7  | 2.307562  | 3.959285  | 0.468872  |
| 1  | 2.400998  | 4.545601  | 1.294400  |
| 1  | 1.652261  | 4.434800  | -0.145799 |
| 1  | 3.210671  | 3.974838  | 0.002100  |
| 7  | 1.847914  | 1.617973  | -4.143607 |
| 1  | 2.841238  | 1.626214  | -4.356246 |
| 1  | 1.474191  | 2.509883  | -4.454445 |
| 1  | 1.427619  | 0.904454  | -4.731776 |
| 7  | -6.148580 | 0.397702  | -0.338679 |
| 1  | -6.869735 | 0.500035  | -1.047112 |
| 1  | -6.284343 | 1.152208  | 0.327809  |
| 1  | -6.344129 | -0.468278 | 0.155002  |
| 7  | 1.965348  | 1.185050  | 2.153257  |
| 1  | 2.032354  | 2.070619  | 1.646685  |
| 1  | 2.227245  | 0.451589  | 1.491886  |
| 1  | 2.683836  | 1.207895  | 2.872575  |

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Cartesian coordinates of : P\_NH3\_N12\_28.log

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.308738 | 0.751959  | 1.084312  |
| 1  | -1.562783 | -0.262581 | 1.000695  |
| 1  | -2.139580 | 1.312122  | 1.346861  |
| 1  | -0.557732 | 0.853521  | 1.811038  |
| 1  | -0.868323 | 1.117004  | 0.194034  |
| 7  | 3.132681  | 0.839299  | 0.260224  |
| 1  | 3.375045  | 0.197768  | -0.496993 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.189001  | 0.288077  | 1.117333  |
| 1 | 3.868095  | 1.539557  | 0.306333  |
| 7 | 0.960967  | -1.363477 | -0.301267 |
| 1 | 1.819150  | -1.518843 | -0.831068 |
| 1 | 0.192539  | -1.286429 | -0.974924 |
| 1 | 1.072192  | -0.434969 | 0.105964  |
| 7 | -1.736667 | -2.109317 | 0.969778  |
| 1 | -0.762053 | -2.317511 | 0.744140  |
| 1 | -1.970476 | -2.583467 | 1.837068  |
| 1 | -2.312340 | -2.513898 | 0.231665  |
| 7 | 1.055864  | 1.128701  | 2.674225  |
| 1 | 1.569589  | 1.749016  | 2.051421  |
| 1 | 1.605636  | 0.266618  | 2.731712  |
| 1 | 1.048150  | 1.554940  | 3.596305  |
| 7 | -1.673374 | -0.934494 | -2.042269 |
| 1 | -2.261050 | -1.736214 | -1.808808 |
| 1 | -2.175328 | -0.102499 | -1.742940 |
| 1 | -1.619846 | -0.891116 | -3.056454 |
| 7 | -3.712591 | 2.360665  | 1.923307  |
| 1 | -4.546170 | 1.787745  | 2.023266  |
| 1 | -3.950046 | 3.111932  | 1.281350  |
| 1 | -3.547795 | 2.793281  | 2.828305  |
| 7 | 0.254493  | 1.699205  | -1.100571 |
| 1 | 0.128699  | 2.628198  | -1.513804 |
| 1 | 0.217564  | 1.015906  | -1.854118 |
| 1 | 1.200784  | 1.649089  | -0.713057 |
| 7 | -3.484280 | -3.604195 | -1.403434 |
| 1 | -3.962191 | -3.481947 | -2.292809 |
| 1 | -4.205560 | -3.847544 | -0.729103 |
| 1 | -2.894343 | -4.426263 | -1.504517 |
| 7 | 2.554892  | -1.644042 | 2.343901  |
| 1 | 1.943559  | -1.958496 | 1.587785  |
| 1 | 2.279324  | -2.136205 | 3.189497  |
| 1 | 3.495504  | -1.962842 | 2.126837  |
| 7 | -0.038792 | 4.568679  | -2.437179 |
| 1 | 0.049776  | 5.322523  | -1.762037 |
| 1 | -0.897260 | 4.737008  | -2.953385 |
| 1 | 0.725462  | 4.676974  | -3.097800 |
| 7 | 3.971673  | -1.639220 | -1.787133 |
| 1 | 3.778765  | -1.457121 | -2.768508 |
| 1 | 3.888412  | -2.644390 | -1.657632 |
| 1 | 4.952727  | -1.415280 | -1.640901 |

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Cartesian coordinates of : P\_NH3\_N12\_24.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.379694  | -0.314488 | 1.530400  |
| 1  | 0.531973  | -0.822269 | 2.417007  |
| 1  | 1.242492  | -0.339444 | 0.902304  |
| 1  | -0.431196 | -0.705731 | 0.987821  |
| 1  | 0.189023  | 0.695030  | 1.697510  |
| 7  | -1.742186 | -1.060890 | -0.248523 |
| 1  | -1.662554 | -1.969916 | -0.707425 |
| 1  | -2.713243 | -0.916600 | 0.022513  |
| 1  | -1.515346 | -0.342239 | -0.938098 |
| 7  | 0.875445  | -1.765511 | 4.144248  |
| 1  | 0.600877  | -1.213994 | 4.952461  |
| 1  | 0.383441  | -2.651840 | 4.214639  |
| 1  | 1.864743  | -1.970929 | 4.253557  |
| 7  | -0.048822 | 2.566139  | 1.381008  |
| 1  | -0.990862 | 2.654120  | 0.997368  |
| 1  | 0.615671  | 2.822742  | 0.650826  |
| 1  | 0.046366  | 3.239901  | 2.134770  |
| 7  | -4.981249 | -0.471481 | 0.333136  |
| 1  | -5.726753 | 0.168365  | 0.596014  |
| 1  | -5.033455 | -1.249279 | 0.985920  |
| 1  | -5.229847 | -0.840376 | -0.581190 |
| 7  | -1.162480 | -3.946623 | -1.701439 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.235618 | -4.344048 | -1.572556 |
| 1 | -1.797928 | -4.515995 | -1.148897 |
| 1 | -1.414332 | -4.097499 | -2.674669 |
| 7 | 2.436964  | -0.071471 | -0.336454 |
| 1 | 3.418891  | -0.333519 | -0.217224 |
| 1 | 2.055732  | -0.560795 | -1.152991 |
| 1 | 2.400220  | 0.925388  | -0.541289 |
| 7 | -0.720078 | 1.616247  | -1.700148 |
| 1 | -0.930532 | 2.087426  | -2.576141 |
| 1 | -1.410123 | 1.935085  | -1.017485 |
| 1 | 0.190184  | 1.957759  | -1.391865 |
| 7 | 2.104188  | 3.311851  | -1.087715 |
| 1 | 2.494873  | 2.993194  | -1.971692 |
| 1 | 2.897586  | 3.518889  | -0.485399 |
| 1 | 1.653108  | 4.202920  | -1.282143 |
| 7 | -3.141901 | 2.244088  | 0.374455  |
| 1 | -3.668906 | 2.802493  | -0.292704 |
| 1 | -3.383258 | 2.607197  | 1.293593  |
| 1 | -3.525528 | 1.297415  | 0.333429  |
| 7 | 0.590918  | -1.207128 | -2.552256 |
| 1 | -0.000754 | -1.977371 | -2.247322 |
| 1 | 0.806056  | -1.357272 | -3.533111 |
| 1 | 0.040254  | -0.351104 | -2.476944 |
| 7 | 5.502911  | -0.927214 | -0.060317 |
| 1 | 5.979220  | -0.759165 | -0.941618 |
| 1 | 5.551543  | -1.926958 | 0.112597  |
| 1 | 6.054160  | -0.476209 | 0.663683  |

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Cartesian coordinates of : P\_NH3\_N12\_19.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.515186 | 0.152357  | 0.292070  |
| 1  | 0.154219  | -0.640934 | 0.141513  |
| 1  | -0.947645 | 0.081822  | 1.242033  |
| 1  | 0.013074  | 1.053683  | 0.208581  |
| 1  | -1.286430 | 0.121098  | -0.411533 |
| 7  | 1.194623  | 2.478641  | 0.070863  |
| 1  | 1.273971  | 3.094114  | 0.875122  |
| 1  | 2.065839  | 1.932592  | 0.002629  |
| 1  | 1.135513  | 3.075574  | -0.748839 |
| 7  | 1.424842  | -1.989044 | -0.075813 |
| 1  | 1.961341  | -1.858264 | -0.936386 |
| 1  | 2.084647  | -1.949457 | 0.704727  |
| 1  | 1.046791  | -2.931994 | -0.100068 |
| 7  | -2.814483 | 0.112812  | -1.540144 |
| 1  | -3.375367 | 0.943425  | -1.341213 |
| 1  | -3.402658 | -0.701563 | -1.354835 |
| 1  | -2.615047 | 0.117378  | -2.536472 |
| 7  | 3.489229  | 0.478957  | -0.114516 |
| 1  | 3.335299  | -0.092391 | -0.943083 |
| 1  | 3.425396  | -0.154022 | 0.680366  |
| 1  | 4.446802  | 0.836894  | -0.153789 |
| 7  | 3.492970  | -1.787219 | 2.424355  |
| 1  | 4.476981  | -1.921776 | 2.207790  |
| 1  | 3.439233  | -1.016904 | 3.085325  |
| 1  | 3.191659  | -2.618375 | 2.926096  |
| 7  | -2.016200 | -0.013338 | 2.777160  |
| 1  | -1.962726 | -0.864003 | 3.329779  |
| 1  | -1.944987 | 0.762283  | 3.429373  |
| 1  | -2.949190 | 0.022893  | 2.347671  |
| 7  | 3.194326  | -1.596755 | -2.785370 |
| 1  | 2.799848  | -2.366971 | -3.318717 |
| 1  | 3.149401  | -0.778240 | -3.386320 |
| 1  | 4.179175  | -1.811479 | -2.653713 |
| 7  | -4.610621 | 0.107119  | 1.102276  |
| 1  | -5.495628 | 0.125837  | 1.600694  |
| 1  | -4.627543 | -0.700320 | 0.480503  |
| 1  | -4.576620 | 0.935475  | 0.509464  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 6.421613  | 1.773310  | -0.227406 |
| 1 | 6.563732  | 2.318758  | 0.617644  |
| 1 | 6.443876  | 2.427422  | -1.004247 |
| 1 | 7.231946  | 1.169374  | -0.327625 |
| 7 | -4.546253 | 2.819863  | -0.843772 |
| 1 | -5.549507 | 2.822285  | -1.008462 |
| 1 | -4.127813 | 3.318060  | -1.625174 |
| 1 | -4.383299 | 3.394328  | -0.020850 |
| 7 | -4.762646 | -2.490739 | -0.984594 |
| 1 | -5.735771 | -2.340965 | -1.238200 |
| 1 | -4.762241 | -3.124801 | -0.189784 |
| 1 | -4.341764 | -3.002577 | -1.755760 |

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Cartesian coordinates of : P\_NH3\_N12\_20.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.444153 | 0.077242  | -0.328404 |
| 1  | -0.020546 | 1.001037  | -0.080312 |
| 1  | -1.038619 | 0.164221  | -1.188985 |
| 1  | 0.377815  | -0.547378 | -0.508353 |
| 1  | -1.022537 | -0.281811 | 0.461196  |
| 7  | 2.136699  | -1.118300 | -0.778733 |
| 1  | 2.395689  | -1.063842 | -1.760796 |
| 1  | 2.691852  | -0.407042 | -0.295535 |
| 1  | 2.467979  | -2.025172 | -0.447505 |
| 7  | 1.207145  | 2.377174  | 0.284295  |
| 1  | 2.113522  | 1.908706  | 0.406278  |
| 1  | 1.317226  | 3.047823  | -0.471394 |
| 1  | 1.033581  | 2.918710  | 1.126546  |
| 7  | -2.069562 | -0.900534 | 1.938838  |
| 1  | -2.046512 | -1.911603 | 2.043517  |
| 1  | -3.058215 | -0.627341 | 1.910605  |
| 1  | -1.685089 | -0.519140 | 2.799539  |
| 7  | 4.008313  | 1.061615  | 0.812928  |
| 1  | 3.998183  | 1.063099  | 1.830204  |
| 1  | 4.513466  | 1.906272  | 0.529041  |
| 1  | 4.579204  | 0.256402  | 0.536915  |
| 7  | 5.575886  | 3.739652  | 0.017737  |
| 1  | 6.506537  | 3.652968  | 0.415621  |
| 1  | 5.694158  | 3.870955  | -0.982348 |
| 1  | 5.178294  | 4.599319  | 0.384182  |
| 7  | -2.212137 | 0.269351  | -2.609452 |
| 1  | -2.377194 | 1.206686  | -2.965103 |
| 1  | -1.983848 | -0.309302 | -3.412909 |
| 1  | -3.096973 | -0.077646 | -2.218147 |
| 7  | 3.216217  | -4.138985 | 0.057231  |
| 1  | 2.289293  | -4.491862 | -0.166388 |
| 1  | 3.872730  | -4.711430 | -0.467352 |
| 1  | 3.372701  | -4.343686 | 1.040669  |
| 7  | -4.647983 | -0.872504 | -1.097385 |
| 1  | -5.064117 | -1.700364 | -1.513773 |
| 1  | -5.402856 | -0.218712 | -0.893183 |
| 1  | -4.266455 | -1.143681 | -0.194462 |
| 7  | 5.400521  | -1.632403 | -0.094906 |
| 1  | 5.756639  | -1.571482 | -1.044226 |
| 1  | 4.694913  | -2.367437 | -0.080721 |
| 1  | 6.173861  | -1.932891 | 0.490955  |
| 7  | -5.147399 | -0.184546 | 2.010251  |
| 1  | -5.708692 | -1.013062 | 2.190867  |
| 1  | -5.627623 | 0.338374  | 1.275936  |
| 1  | -5.192847 | 0.378690  | 2.855487  |
| 7  | -6.973875 | 1.351170  | -0.272941 |
| 1  | -7.287072 | 1.997767  | 0.446785  |
| 1  | -7.796743 | 0.828134  | -0.561563 |
| 1  | -6.699398 | 1.923196  | -1.067499 |

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Cartesian coordinates of : P\_NH3\_N12\_14.log

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | -0.491062  | 0.555527  | -0.027629 |
| 1  | -0.076976  | 1.247048  | -0.697179 |
| 1  | 0.215923   | 0.453788  | 0.738684  |
| 1  | -1.410119  | 0.884077  | 0.341328  |
| 1  | -0.695932  | -0.354760 | -0.492238 |
| 7  | -3.255244  | 0.981022  | 0.770167  |
| 1  | -3.743052  | 1.809056  | 0.439465  |
| 1  | -3.695061  | 0.180039  | 0.310146  |
| 1  | -3.462741  | 0.901756  | 1.761996  |
| 7  | 1.036507   | 2.465314  | -1.558485 |
| 1  | 1.186576   | 2.275598  | -2.545625 |
| 1  | 0.744695   | 3.436719  | -1.493951 |
| 1  | 1.948096   | 2.387341  | -1.091523 |
| 7  | -1.646199  | -1.863556 | -1.165901 |
| 1  | -1.403668  | -2.748566 | -0.729398 |
| 1  | -1.565660  | -2.002953 | -2.169259 |
| 1  | -2.634255  | -1.684521 | -0.962115 |
| 7  | -4.798035  | -1.494062 | -0.673081 |
| 1  | -4.959233  | -2.379694 | -0.199204 |
| 1  | -5.005419  | -1.659631 | -1.655268 |
| 1  | -5.521951  | -0.845951 | -0.331762 |
| 7  | 9.143067   | -2.019689 | 0.079298  |
| 1  | 8.900236   | -2.982836 | -0.132767 |
| 1  | 9.959892   | -1.791229 | -0.479713 |
| 1  | 9.435933   | -1.996637 | 1.051592  |
| 7  | 1.706607   | 0.693632  | 1.828987  |
| 1  | 1.598289   | 0.565412  | 2.831145  |
| 1  | 2.506358   | 0.126052  | 1.529561  |
| 1  | 1.976240   | 1.663194  | 1.678116  |
| 7  | 6.785983   | -0.008530 | -0.536939 |
| 1  | 7.541959   | -0.669268 | -0.328638 |
| 1  | 6.732107   | 0.062493  | -1.549372 |
| 1  | 7.089861   | 0.900447  | -0.198539 |
| 7  | 3.845298   | 2.076496  | -0.192080 |
| 1  | 3.995979   | 1.133393  | 0.170231  |
| 1  | 4.188078   | 2.723386  | 0.513583  |
| 1  | 4.467192   | 2.178245  | -0.990089 |
| 7  | -6.872174  | 0.531407  | 0.393488  |
| 1  | -6.927066  | 1.396308  | -0.137521 |
| 1  | -6.753112  | 0.798454  | 1.366799  |
| 1  | -7.791456  | 0.082682  | 0.320371  |
| 7  | 4.243407   | -0.997155 | 0.918669  |
| 1  | 4.523638   | -1.357664 | 1.827404  |
| 1  | 5.109719   | -0.738432 | 0.427250  |
| 1  | 3.842595   | -1.782578 | 0.412481  |
| 7  | -9.716581  | -0.818974 | 0.168615  |
| 1  | -9.984982  | -0.991254 | -0.795759 |
| 1  | -10.431595 | -0.219737 | 0.570613  |
| 1  | -9.772102  | -1.709802 | 0.653394  |

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Cartesian coordinates of : P\_NH3\_N12\_17.log-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.033923 | -0.059827 | 0.154920  |
| 1  | -0.576909 | -0.371141 | -0.685130 |
| 1  | 0.788773  | 0.511242  | -0.132709 |
| 1  | -0.660851 | 0.490887  | 0.799112  |
| 1  | 0.375776  | -0.878749 | 0.651557  |
| 7  | -1.857786 | 1.413180  | 1.805033  |
| 1  | -1.708512 | 2.417533  | 1.847619  |
| 1  | -2.752660 | 1.252836  | 1.317646  |
| 1  | -1.966567 | 1.096994  | 2.764587  |
| 7  | -1.520223 | -0.908973 | -2.209062 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -2.485364 | -1.204365 | -2.014666 |
| 1 | -1.574505 | -0.169111 | -2.904665 |
| 1 | -1.062512 | -1.692731 | -2.667722 |
| 7 | 1.646058  | -2.085133 | 1.430355  |
| 1 | 1.590820  | -2.154696 | 2.442610  |
| 1 | 2.570033  | -1.706712 | 1.201349  |
| 1 | 1.610974  | -3.035230 | 1.071785  |
| 7 | -4.312296 | 0.793224  | 0.111190  |
| 1 | -4.808055 | -0.051846 | 0.388590  |
| 1 | -3.944403 | 0.602730  | -0.817308 |
| 1 | -4.998980 | 1.547302  | 0.025272  |
| 7 | -4.481316 | -1.831528 | -1.810265 |
| 1 | -4.847498 | -1.909941 | -0.859264 |
| 1 | -5.143779 | -1.262170 | -2.330685 |
| 1 | -4.517882 | -2.759536 | -2.223649 |
| 7 | 2.587111  | 1.128792  | -0.361514 |
| 1 | 2.894290  | 1.275976  | -1.319010 |
| 1 | 2.798056  | 1.985625  | 0.142842  |
| 1 | 3.188576  | 0.399513  | 0.029397  |
| 7 | 9.307148  | 0.473758  | -0.206713 |
| 1 | 9.888308  | 1.175545  | -0.655757 |
| 1 | 9.533640  | 0.493143  | 0.783230  |
| 1 | 9.609491  | -0.429141 | -0.560384 |
| 7 | 4.643129  | -1.100734 | 0.820505  |
| 1 | 5.212490  | -0.419399 | 0.298905  |
| 1 | 4.910748  | -2.019201 | 0.474325  |
| 1 | 4.961221  | -1.061409 | 1.785993  |
| 7 | -6.394666 | 3.209133  | -0.090159 |
| 1 | -5.974143 | 3.992870  | -0.580696 |
| 1 | -6.631703 | 3.538546  | 0.840965  |
| 1 | -7.269933 | 3.002663  | -0.562129 |
| 7 | 6.246830  | 1.006341  | -0.772046 |
| 1 | 6.129908  | 0.953260  | -1.780244 |
| 1 | 7.238996  | 0.830933  | -0.580975 |
| 1 | 6.064015  | 1.971467  | -0.511498 |
| 7 | -5.862972 | -2.029955 | 1.131990  |
| 1 | -5.392846 | -1.873216 | 2.019440  |
| 1 | -6.050829 | -3.027643 | 1.077959  |
| 1 | -6.767846 | -1.570769 | 1.193677  |

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Cartesian coordinates of : P\_NH3\_N12\_11.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.734050  | -0.117599 | 0.313626  |
| 1  | 1.187291  | 0.358581  | 1.067439  |
| 1  | 2.525069  | -0.657763 | 0.732334  |
| 1  | 1.050592  | -0.769814 | -0.148525 |
| 1  | 2.099967  | 0.577445  | -0.374587 |
| 7  | -0.431220 | -1.750196 | -0.627281 |
| 1  | -0.306378 | -2.740259 | -0.816916 |
| 1  | -1.069675 | -1.660431 | 0.162841  |
| 1  | -0.937906 | -1.342088 | -1.419495 |
| 7  | -0.177338 | 0.827286  | 2.280515  |
| 1  | 0.046094  | 0.791241  | 3.270794  |
| 1  | -0.640608 | 1.719875  | 2.101562  |
| 1  | -0.892916 | 0.124319  | 2.091761  |
| 7  | 2.759398  | 1.804940  | -1.656948 |
| 1  | 3.051996  | 1.326544  | -2.504939 |
| 1  | 3.563183  | 2.354303  | -1.333095 |
| 1  | 2.042781  | 2.468915  | -1.937887 |
| 7  | 3.942716  | -1.618396 | 1.527779  |
| 1  | 3.679732  | -1.987973 | 2.437659  |
| 1  | 4.255932  | -2.416062 | 0.963198  |
| 1  | 4.757501  | -1.031033 | 1.684569  |
| 7  | 5.224061  | 3.554054  | -0.778844 |
| 1  | 5.317021  | 4.330919  | -1.427074 |
| 1  | 5.145107  | 3.955668  | 0.150833  |
| 1  | 6.103127  | 3.045611  | -0.805157 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 4.981728  | -4.089665 | -0.113713 |
| 1 | 5.088965  | -3.919509 | -1.109361 |
| 1 | 4.379020  | -4.901759 | -0.017856 |
| 1 | 5.895537  | -4.360849 | 0.238023  |
| 7 | -2.674744 | 0.075255  | 0.590894  |
| 1 | -2.535648 | 0.048271  | -0.419262 |
| 1 | -2.597594 | 1.049951  | 0.878216  |
| 1 | -3.635749 | -0.221669 | 0.752545  |
| 7 | -5.476564 | -1.532496 | 1.300988  |
| 1 | -4.926349 | -2.387184 | 1.285997  |
| 1 | -6.447626 | -1.807563 | 1.178588  |
| 1 | -5.403116 | -1.155525 | 2.242194  |
| 7 | -2.145892 | 3.359570  | 1.600004  |
| 1 | -1.530949 | 4.113419  | 1.895235  |
| 1 | -2.939351 | 3.371913  | 2.235303  |
| 1 | -2.499584 | 3.622047  | 0.684006  |
| 7 | -2.354864 | -0.399395 | -2.766769 |
| 1 | -2.302249 | -1.083497 | -3.517225 |
| 1 | -2.111904 | 0.495021  | -3.183824 |
| 1 | -3.340812 | -0.342893 | -2.485223 |
| 7 | -5.267827 | -0.183887 | -1.664053 |
| 1 | -5.594550 | 0.777598  | -1.631660 |
| 1 | -5.343740 | -0.559429 | -0.717597 |
| 1 | -5.926745 | -0.692646 | -2.246792 |

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Cartesian coordinates of : P\_NH3\_N12\_22.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.315490  | -0.063597 | 1.032570  |
| 1  | 0.210957  | -1.101322 | 1.020175  |
| 1  | 1.135542  | 0.233084  | 0.419270  |
| 1  | -0.596784 | 0.299776  | 0.659309  |
| 1  | 0.473817  | 0.263155  | 2.000514  |
| 7  | -2.311014 | 0.340675  | -0.037368 |
| 1  | -2.420507 | 0.693840  | -0.989516 |
| 1  | -2.538776 | -0.654443 | -0.089576 |
| 1  | -3.066111 | 0.764634  | 0.504102  |
| 7  | -0.438686 | -2.881697 | 0.787077  |
| 1  | -0.490985 | -3.438818 | 1.635381  |
| 1  | -1.390834 | -2.814424 | 0.410356  |
| 1  | 0.109513  | -3.420721 | 0.122359  |
| 7  | 0.936632  | 0.854103  | 3.852006  |
| 1  | 0.574705  | 1.774210  | 4.086082  |
| 1  | 1.947550  | 0.905243  | 3.943732  |
| 1  | 0.608627  | 0.217938  | 4.573320  |
| 7  | -3.397459 | -2.854068 | -0.368181 |
| 1  | -3.881435 | -3.374773 | 0.359200  |
| 1  | -3.269450 | -3.504651 | -1.139428 |
| 1  | -4.052886 | -2.134208 | -0.698147 |
| 7  | -2.921159 | 1.277639  | -3.188358 |
| 1  | -2.013619 | 1.730758  | -3.254138 |
| 1  | -2.941494 | 0.567413  | -3.915337 |
| 1  | -3.611075 | 1.979057  | -3.443888 |
| 7  | 2.543778  | 0.677598  | -0.536293 |
| 1  | 2.469804  | 0.373921  | -1.503865 |
| 1  | 2.723005  | 1.685686  | -0.560505 |
| 1  | 3.381704  | 0.222829  | -0.152063 |
| 7  | -5.029239 | 1.512342  | 1.533588  |
| 1  | -4.474106 | 2.015329  | 2.220648  |
| 1  | -5.651851 | 2.197021  | 1.112917  |
| 1  | -5.614711 | 0.865603  | 2.055504  |
| 7  | 5.074152  | -0.769186 | 0.619447  |
| 1  | 5.618560  | -0.186259 | 1.248976  |
| 1  | 5.694286  | -1.028040 | -0.153642 |
| 1  | 4.865534  | -1.623560 | 1.128187  |
| 7  | -5.084549 | -0.401125 | -1.235046 |
| 1  | -4.485254 | 0.103338  | -1.886768 |
| 1  | -5.140041 | 0.171517  | -0.394015 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -6.013785 | -0.460454 | -1.639878 |
| 7 | 3.213369  | 3.804947  | -0.696496 |
| 1 | 2.477719  | 4.468305  | -0.472929 |
| 1 | 3.525628  | 4.017007  | -1.639526 |
| 1 | 3.992672  | 4.007660  | -0.077388 |
| 7 | 7.077756  | -1.599511 | -1.703649 |
| 1 | 6.713132  | -2.319591 | -2.320064 |
| 1 | 7.931161  | -1.966953 | -1.293152 |
| 1 | 7.346299  | -0.815933 | -2.291281 |

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Cartesian coordinates of : P\_NH3\_N12\_27.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.083050 | 0.314918  | -0.150735 |
| 1  | -1.895271 | 0.324378  | -0.803247 |
| 1  | -0.807802 | -0.693420 | 0.083176  |
| 1  | -0.243768 | 0.713212  | -0.619670 |
| 1  | -1.317734 | 0.847555  | 0.712398  |
| 7  | 1.491309  | 0.741387  | -1.470076 |
| 1  | 1.422046  | 0.554864  | -2.467235 |
| 1  | 2.149539  | 1.513290  | -1.368015 |
| 1  | 1.934012  | -0.080837 | -1.051086 |
| 7  | -3.368394 | 0.259261  | -2.028218 |
| 1  | -3.791558 | -0.664809 | -2.004471 |
| 1  | -4.118862 | 0.934190  | -1.846524 |
| 1  | -3.064827 | 0.409443  | -2.986683 |
| 7  | -1.872776 | 1.800170  | 2.287165  |
| 1  | -1.105867 | 2.063687  | 2.914765  |
| 1  | -2.514320 | 1.228340  | 2.830137  |
| 1  | -2.374658 | 2.654346  | 2.059947  |
| 7  | 3.176134  | -1.704527 | -0.183035 |
| 1  | 3.364655  | -1.890221 | 0.798454  |
| 1  | 3.867474  | -1.013712 | -0.496754 |
| 1  | 3.372015  | -2.568735 | -0.681159 |
| 7  | 0.404483  | 2.652942  | 4.295847  |
| 1  | 0.123908  | 2.449412  | 5.250752  |
| 1  | 1.288023  | 2.177249  | 4.139257  |
| 1  | 0.593609  | 3.650060  | 4.253176  |
| 7  | -0.053319 | -2.245302 | 0.286842  |
| 1  | -0.377771 | -2.951033 | -0.379364 |
| 1  | 0.939106  | -2.085113 | 0.102696  |
| 1  | -0.132204 | -2.651307 | 1.222669  |
| 7  | -5.758176 | 2.278066  | -1.620029 |
| 1  | -6.394938 | 2.154794  | -2.402104 |
| 1  | -6.298976 | 2.120242  | -0.774797 |
| 1  | -5.484606 | 3.256279  | -1.616498 |
| 7  | -0.349862 | -3.661651 | 3.167098  |
| 1  | 0.183987  | -4.525636 | 3.159016  |
| 1  | -1.321170 | -3.916214 | 3.319407  |
| 1  | -0.050226 | -3.136785 | 3.983035  |
| 7  | -1.010402 | -4.558612 | -1.749168 |
| 1  | -0.436969 | -5.370863 | -1.541529 |
| 1  | -0.891628 | -4.358971 | -2.737737 |
| 1  | -1.977373 | -4.839654 | -1.617654 |
| 7  | 3.394099  | 3.471282  | -1.561124 |
| 1  | 4.150125  | 3.946159  | -1.074724 |
| 1  | 2.533783  | 3.925395  | -1.265714 |
| 1  | 3.509151  | 3.681954  | -2.548994 |
| 7  | 4.978126  | 0.587813  | -1.299543 |
| 1  | 5.832914  | 0.772788  | -0.782958 |
| 1  | 4.444538  | 1.456239  | -1.336119 |
| 1  | 5.254440  | 0.363214  | -2.251025 |

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Cartesian coordinates of : P\_NH3\_N12\_33.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.650667 | 0.133128  | -0.088946 |
| 1  | 0.036237  | -0.508069 | 0.437802  |
| 1  | -1.205573 | -0.449133 | -0.748605 |
| 1  | -1.286105 | 0.608192  | 0.582974  |
| 1  | -0.100144 | 0.840354  | -0.620757 |
| 7  | 3.111644  | 3.419890  | 0.579281  |
| 1  | 4.063179  | 3.633345  | 0.292312  |
| 1  | 3.160704  | 3.087055  | 1.538518  |
| 1  | 2.615404  | 4.306669  | 0.607585  |
| 7  | 3.389546  | 0.242120  | -0.455265 |
| 1  | 4.380905  | 0.025902  | -0.409553 |
| 1  | 3.118290  | 0.224498  | -1.436664 |
| 1  | 3.270086  | 1.202042  | -0.136304 |
| 7  | 1.252289  | -1.484871 | 1.130753  |
| 1  | 2.096076  | -1.070919 | 0.724909  |
| 1  | 1.339763  | -1.457622 | 2.148942  |
| 1  | 1.216925  | -2.467704 | 0.852016  |
| 7  | -2.454486 | 1.417038  | 1.900955  |
| 1  | -3.129565 | 0.734836  | 2.235630  |
| 1  | -2.987589 | 2.231037  | 1.578408  |
| 1  | -1.922835 | 1.714126  | 2.714676  |
| 7  | 2.833632  | 0.463003  | -3.775150 |
| 1  | 3.758233  | 0.867122  | -3.898588 |
| 1  | 2.941221  | -0.544977 | -3.850606 |
| 1  | 2.283307  | 0.753037  | -4.579232 |
| 7  | -2.068892 | -1.717208 | -1.923511 |
| 1  | -1.951757 | -1.495467 | -2.908316 |
| 1  | -3.071387 | -1.865757 | -1.769196 |
| 1  | -1.609328 | -2.611432 | -1.772000 |
| 7  | 1.022009  | 2.076416  | -1.572638 |
| 1  | 0.526795  | 2.823278  | -2.051387 |
| 1  | 1.572558  | 1.579642  | -2.275549 |
| 1  | 1.679203  | 2.515580  | -0.925337 |
| 7  | 1.279206  | -4.658310 | 0.425280  |
| 1  | 1.322509  | -4.986265 | -0.534694 |
| 1  | 0.539917  | -5.181309 | 0.884783  |
| 1  | 2.152484  | -4.929051 | 0.867930  |
| 7  | 1.596538  | -1.588330 | 4.352213  |
| 1  | 2.550828  | -1.890881 | 4.523306  |
| 1  | 0.985543  | -2.302890 | 4.736139  |
| 1  | 1.449623  | -0.747377 | 4.901825  |
| 7  | -4.162005 | 3.927327  | 1.018724  |
| 1  | -4.951048 | 4.034633  | 1.649590  |
| 1  | -4.542947 | 3.854448  | 0.080025  |
| 1  | -3.637134 | 4.796144  | 1.056186  |
| 7  | -5.159196 | -2.269752 | -1.570893 |
| 1  | -5.403020 | -2.688616 | -0.678277 |
| 1  | -5.456794 | -2.920555 | -2.292002 |
| 1  | -5.731892 | -1.437066 | -1.672122 |

Cartesian coordinates of : P\_NH3\_N12\_12.log

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.727538 | 0.020882  | -0.086118 |
| 1  | -1.186500 | -0.343016 | -0.907390 |
| 1  | -2.231490 | -0.760160 | 0.389652  |
| 1  | -0.997577 | 0.432061  | 0.547777  |
| 1  | -2.411275 | 0.749143  | -0.390853 |
| 7  | 0.620406  | 0.983586  | 1.253111  |
| 1  | 0.858212  | 0.729555  | 2.212361  |
| 1  | 1.307743  | 0.527796  | 0.644209  |
| 1  | 0.783877  | 1.983833  | 1.172718  |
| 7  | 0.185310  | -0.816515 | -2.068700 |
| 1  | 0.236665  | -1.798931 | -2.324217 |
| 1  | 0.226637  | -0.290020 | -2.936976 |
| 1  | 1.044563  | -0.604577 | -1.543053 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -3.714068 | 2.002224  | -0.960628 |
| 1 | -3.999394 | 1.822542  | -1.919808 |
| 1 | -3.403119 | 2.979324  | -0.923436 |
| 1 | -4.558299 | 1.942399  | -0.397274 |
| 7 | -3.147105 | -2.185984 | 1.242227  |
| 1 | -3.612155 | -1.899144 | 2.099446  |
| 1 | -3.864735 | -2.610160 | 0.643653  |
| 1 | -2.503976 | -2.929395 | 1.501640  |
| 7 | -2.916251 | 5.044139  | -0.911542 |
| 1 | -3.662489 | 5.567181  | -1.360880 |
| 1 | -2.813409 | 5.425993  | 0.024104  |
| 1 | -2.061142 | 5.262224  | -1.414448 |
| 7 | -5.365963 | -3.569876 | -0.503058 |
| 1 | -5.101631 | -3.722787 | -1.471857 |
| 1 | -6.243147 | -3.057649 | -0.515642 |
| 1 | -5.567265 | -4.483340 | -0.106266 |
| 7 | 2.881927  | -0.389811 | -0.600588 |
| 1 | 3.270303  | -0.315784 | 0.343329  |
| 1 | 3.382968  | 0.285100  | -1.183190 |
| 1 | 3.121502  | -1.319534 | -0.952702 |
| 7 | 3.629415  | -3.305453 | -1.853175 |
| 1 | 3.181360  | -4.132181 | -1.470119 |
| 1 | 4.617482  | -3.374480 | -1.627727 |
| 1 | 3.552894  | -3.365847 | -2.863941 |
| 7 | 4.603005  | 1.655994  | -2.466793 |
| 1 | 4.414010  | 2.650127  | -2.384433 |
| 1 | 4.560324  | 1.426481  | -3.454989 |
| 1 | 5.563338  | 1.510719  | -2.170029 |
| 7 | 3.740656  | 0.132783  | 2.444611  |
| 1 | 2.913827  | 0.242416  | 3.029538  |
| 1 | 4.257045  | 1.006570  | 2.478825  |
| 1 | 4.329862  | -0.576450 | 2.870028  |
| 7 | 1.143321  | 0.413190  | 4.484363  |
| 1 | 1.713819  | 0.951302  | 5.131386  |
| 1 | 1.160839  | -0.549045 | 4.811648  |
| 1 | 0.188531  | 0.741622  | 4.602943  |

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Cartesian coordinates of : P\_NH3\_N12\_25.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.875181 | 0.058303  | 0.926835  |
| 1  | -0.388509 | -0.858518 | 1.023787  |
| 1  | -0.190382 | 0.667292  | 0.429388  |
| 1  | -1.788181 | -0.050619 | 0.357938  |
| 1  | -1.085969 | 0.442415  | 1.862443  |
| 7  | -3.232661 | -0.244370 | -0.509044 |
| 1  | -3.061615 | -0.359153 | -1.511652 |
| 1  | -3.740266 | -1.075552 | -0.193530 |
| 1  | -3.865128 | 0.553092  | -0.402128 |
| 7  | 0.923816  | -2.248533 | 0.961221  |
| 1  | 1.056300  | -2.786456 | 1.813108  |
| 1  | 0.769786  | -2.922224 | 0.216197  |
| 1  | 1.812885  | -1.774266 | 0.762073  |
| 7  | -1.542332 | 1.113523  | 3.698245  |
| 1  | -1.846631 | 2.082908  | 3.694679  |
| 1  | -0.763815 | 1.052316  | 4.348351  |
| 1  | -2.302046 | 0.569866  | 4.098142  |
| 7  | -4.855903 | -2.864397 | 0.449892  |
| 1  | -5.683397 | -2.613389 | 0.982507  |
| 1  | -4.334305 | -3.531447 | 1.010336  |
| 1  | -5.177010 | -3.360091 | -0.376380 |
| 7  | -2.815790 | -0.628328 | -3.690174 |
| 1  | -2.186224 | -1.378997 | -3.957123 |
| 1  | -3.730191 | -0.862412 | -4.065254 |
| 1  | -2.503292 | 0.207622  | -4.174631 |
| 7  | 1.400903  | 1.194380  | -0.492791 |
| 1  | 1.284964  | 1.074243  | -1.495868 |
| 1  | 1.843418  | 2.104548  | -0.363141 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 2.081877  | 0.491569  | -0.193909 |
| 7 | -5.332065 | 2.205004  | -0.289251 |
| 1 | -4.955015 | 3.137147  | -0.430879 |
| 1 | -5.984983 | 2.032197  | -1.047919 |
| 1 | -5.876973 | 2.232687  | 0.567214  |
| 7 | 3.725164  | -0.884383 | 0.538913  |
| 1 | 3.999752  | -0.742074 | 1.508082  |
| 1 | 4.164884  | -0.127357 | 0.006165  |
| 1 | 4.162460  | -1.761813 | 0.242647  |
| 7 | 4.704415  | 1.678526  | -1.039724 |
| 1 | 5.642480  | 1.999647  | -0.819634 |
| 1 | 4.056087  | 2.432693  | -0.817031 |
| 1 | 4.670223  | 1.535068  | -2.044649 |
| 7 | 5.121402  | -3.650784 | -0.283388 |
| 1 | 6.119460  | -3.519519 | -0.147398 |
| 1 | 4.987576  | -3.907416 | -1.256799 |
| 1 | 4.851160  | -4.454927 | 0.274840  |
| 7 | 2.744709  | 4.224098  | -0.205554 |
| 1 | 3.214529  | 4.430975  | 0.671893  |
| 1 | 1.792800  | 4.568561  | -0.111612 |
| 1 | 3.187948  | 4.800121  | -0.916505 |

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Cartesian coordinates of : P\_NH3\_N12\_15.log

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Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | -0.000008  | 2.194066  | -0.139322 |
| 1  | -0.000014  | 3.225966  | -0.283094 |
| 1  | 0.886026   | 1.893020  | 0.393349  |
| 1  | -0.886034  | 1.893011  | 0.393356  |
| 1  | -0.000010  | 1.739119  | -1.050542 |
| 7  | -2.315610  | 1.375478  | 1.172020  |
| 1  | -2.835259  | 2.122933  | 1.625710  |
| 1  | -2.949955  | 0.951632  | 0.470923  |
| 1  | -2.154446  | 0.669989  | 1.886881  |
| 7  | -0.000024  | 5.127847  | -0.560218 |
| 1  | -0.814938  | 5.446539  | -1.078010 |
| 1  | -0.000022  | 5.636159  | 0.320314  |
| 1  | 0.814879   | 5.446549  | -1.078021 |
| 7  | -11.355239 | -2.844391 | 0.305505  |
| 1  | -12.109500 | -3.047076 | -0.343569 |
| 1  | -11.735852 | -2.236077 | 1.024017  |
| 1  | -11.108000 | -3.719575 | 0.757262  |
| 7  | -4.176227  | 0.128741  | -0.838078 |
| 1  | -3.831654  | -0.697769 | -1.319022 |
| 1  | -4.546528  | 0.742021  | -1.559141 |
| 1  | -4.978944  | -0.174192 | -0.267433 |
| 7  | 11.355246  | -2.844378 | 0.305521  |
| 1  | 11.108033  | -3.719594 | 0.757231  |
| 1  | 12.109542  | -3.046997 | -0.343532 |
| 1  | 11.735798  | -2.236074 | 1.024074  |
| 7  | 2.315606   | 1.375502  | 1.172003  |
| 1  | 2.835246   | 2.122957  | 1.625704  |
| 1  | 2.154441   | 0.670006  | 1.886857  |
| 1  | 2.949961   | 0.951666  | 0.470908  |
| 7  | 8.862124   | -1.509068 | -1.148111 |
| 1  | 9.661364   | -1.941387 | -0.676639 |
| 1  | 8.539538   | -2.164966 | -1.853587 |
| 1  | 9.212970   | -0.697087 | -1.647658 |
| 7  | 4.176252   | 0.128797  | -0.838083 |
| 1  | 4.978967   | -0.174143 | -0.267439 |
| 1  | 4.546553   | 0.742095  | -1.559130 |
| 1  | 3.831688   | -0.697705 | -1.319047 |
| 7  | -6.584437  | -0.776820 | 0.855777  |
| 1  | -6.951862  | -0.073121 | 1.489932  |
| 1  | -6.405024  | -1.603416 | 1.418858  |
| 1  | -7.340878  | -1.017297 | 0.203414  |
| 7  | 6.584455   | -0.776788 | 0.855767  |
| 1  | 6.951901   | -0.073085 | 1.489904  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 7.340886  | -1.017298 | 0.203404  |
| 1 | 6.405025  | -1.603367 | 1.418867  |
| 7 | -8.862136 | -1.509013 | -1.148101 |
| 1 | -9.212992 | -0.697015 | -1.647613 |
| 1 | -9.661367 | -1.941355 | -0.676636 |
| 1 | -8.539554 | -2.164882 | -1.853606 |

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Cartesian coordinates of : P\_NH3\_N12\_35.log

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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|   |            |           |           |
|---|------------|-----------|-----------|
| 7 | 3.520577   | -0.448156 | 0.427076  |
| 1 | 3.653290   | -0.614562 | 1.423429  |
| 1 | 2.618192   | 0.185490  | 0.269802  |
| 1 | 4.424851   | 0.022398  | 0.017799  |
| 1 | 3.374713   | -1.350391 | -0.023485 |
| 7 | 5.796935   | 0.695960  | -0.554828 |
| 1 | 5.858315   | 1.695231  | -0.372672 |
| 1 | 6.621560   | 0.255024  | -0.101804 |
| 1 | 5.916882   | 0.583646  | -1.559060 |
| 7 | -10.823371 | -1.019523 | -0.359892 |
| 1 | -11.718983 | -0.556296 | -0.186627 |
| 1 | -10.834338 | -1.348959 | -1.320633 |
| 1 | -10.790884 | -1.845778 | 0.229918  |
| 7 | -8.319170  | 0.797279  | 0.150165  |
| 1 | -9.152094  | 0.219631  | -0.009896 |
| 1 | -8.366783  | 1.579016  | -0.496757 |
| 1 | -8.399756  | 1.189804  | 1.083590  |
| 7 | 8.181745   | -0.559864 | 0.727089  |
| 1 | 8.243456   | -1.572788 | 0.668192  |
| 1 | 8.326993   | -0.323773 | 1.705134  |
| 1 | 8.988624   | -0.183566 | 0.209053  |
| 7 | -3.317255  | 0.744155  | 0.609998  |
| 1 | -4.131571  | 0.176228  | 0.336960  |
| 1 | -3.360566  | 0.851568  | 1.619625  |
| 1 | -3.463007  | 1.670906  | 0.219176  |
| 7 | 1.294161   | 1.025412  | 0.021947  |
| 1 | 0.997746   | 1.583146  | 0.820008  |
| 1 | 1.364034   | 1.668189  | -0.763856 |
| 1 | 0.514752   | 0.366376  | -0.189237 |
| 7 | -5.766262  | -0.949146 | -0.210625 |
| 1 | -6.604726  | -0.366773 | -0.091584 |
| 1 | -5.757455  | -1.261929 | -1.177262 |
| 1 | -5.900516  | -1.780697 | 0.357645  |
| 7 | -0.948314  | -0.815437 | -0.516097 |
| 1 | -1.747315  | -0.288152 | -0.129546 |
| 1 | -0.960363  | -1.729047 | -0.070596 |
| 1 | -1.155209  | -0.978287 | -1.498150 |
| 7 | 10.588906  | 0.580947  | -0.833512 |
| 1 | 10.646635  | 1.594614  | -0.792544 |
| 1 | 10.586691  | 0.333923  | -1.819157 |
| 1 | 11.461062  | 0.216897  | -0.437522 |
| 7 | 13.318482  | -0.511737 | 0.346330  |
| 1 | 13.452726  | -0.267533 | 1.322961  |
| 1 | 14.102092  | -0.118849 | -0.166844 |
| 1 | 13.398938  | -1.522025 | 0.280570  |
| 7 | -13.593364 | 0.457967  | 0.179482  |
| 1 | -13.619001 | 1.344758  | -0.314366 |
| 1 | -13.715809 | 0.662343  | 1.166492  |
| 1 | -14.404669 | -0.074778 | -0.118683 |

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Cartesian coordinates of the protonated ammonia tridecamer

Cartesian coordinates of : Ca13\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.210435 | -1.096611 | -2.010558 |
| 1  | -0.150158 | 0.628485  | -2.554743 |
| 1  | -1.132504 | -1.567056 | -2.909605 |
| 1  | -0.828212 | -1.743319 | -1.318030 |
| 1  | -2.206912 | -1.004011 | -1.811699 |
| 7  | 2.170544  | -1.378084 | -1.373424 |
| 1  | 2.537836  | -1.908699 | -2.160117 |
| 1  | 1.715712  | -0.556672 | -1.770146 |
| 1  | 1.420730  | -1.944951 | -0.965154 |
| 7  | 1.769145  | 1.660498  | -0.023502 |
| 1  | 2.791088  | 1.469120  | 0.005913  |
| 1  | 1.507515  | 2.612319  | 0.301467  |
| 1  | 1.259847  | 0.938805  | 0.557432  |
| 7  | 0.477598  | 1.436989  | -2.628116 |
| 1  | 1.427239  | 1.575428  | -1.005857 |
| 1  | 0.906628  | 1.428411  | -3.549196 |
| 1  | -0.104267 | 2.270304  | -2.580069 |
| 7  | 0.011688  | -3.175573 | 0.201759  |
| 1  | 0.693534  | -3.162477 | 0.960596  |
| 1  | -0.075114 | -4.137880 | -0.112793 |
| 1  | -0.889640 | -2.896479 | 0.594947  |
| 7  | 2.818300  | -2.295132 | 1.633175  |
| 1  | 3.395737  | -1.759282 | 2.275237  |
| 1  | 2.961486  | -1.924251 | 0.692795  |
| 1  | 3.180118  | -3.244778 | 1.649046  |
| 7  | 4.457638  | 0.566368  | -0.253439 |
| 1  | 4.035445  | -0.283243 | -0.632678 |
| 1  | 5.047133  | 0.305991  | 0.531504  |
| 1  | 5.072742  | 0.954051  | -0.963123 |
| 7  | 0.381365  | -0.338204 | 1.466700  |
| 1  | -0.287108 | -0.844833 | 0.886135  |
| 1  | -0.156340 | 0.000647  | 2.262347  |
| 1  | 1.050303  | -1.036223 | 1.800121  |
| 7  | -2.622653 | -1.463363 | 0.977791  |
| 1  | -3.233043 | -2.167296 | 1.385467  |
| 1  | -3.124061 | -1.061190 | 0.184611  |
| 1  | -2.513331 | -0.725883 | 1.673675  |
| 7  | -4.447376 | -0.529732 | -1.613078 |
| 1  | -4.812668 | -1.431017 | -1.911861 |
| 1  | -4.406020 | 0.051537  | -2.446788 |
| 1  | -5.161646 | -0.119289 | -1.016589 |
| 7  | -2.165426 | 1.030657  | 3.218359  |
| 1  | -3.127290 | 1.355939  | 3.152413  |
| 1  | -1.611476 | 1.843995  | 3.477374  |
| 1  | -2.136052 | 0.402854  | 4.018819  |
| 7  | 0.298275  | 4.099399  | 0.469642  |
| 1  | -0.516253 | 3.528441  | 0.228040  |
| 1  | 0.382150  | 4.845333  | -0.214622 |
| 1  | 0.123950  | 4.544470  | 1.365458  |
| 7  | -1.599207 | 1.613220  | -0.065409 |
| 1  | -1.188840 | 0.828364  | -0.572618 |
| 1  | -2.550331 | 1.701164  | -0.416115 |
| 1  | -1.674126 | 1.320145  | 0.909105  |

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Cartesian coordinates of : BCa13\_2

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.322219  | -0.964867 | 0.049165  |
| 1  | -0.028239 | -0.161805 | 0.652402  |
| 1  | 0.880542  | -0.525887 | -0.708905 |
| 1  | 0.912341  | -1.618923 | 0.607243  |
| 1  | -0.496476 | -1.478605 | -0.351048 |
| 7  | -4.747127 | -1.831705 | 0.588861  |
| 1  | -5.520542 | -1.738984 | -0.064556 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -4.974631 | -1.254252 | 1.394086  |
| 1 | -4.760795 | -2.793851 | 0.917345  |
| 7 | -3.062043 | 0.777315  | -0.676912 |
| 1 | -3.871638 | 1.292673  | -1.013035 |
| 1 | -2.587324 | 0.395846  | -1.497106 |
| 1 | -3.424011 | -0.019420 | -0.153592 |
| 7 | -0.640904 | 1.334583  | 1.352337  |
| 1 | -1.551533 | 1.405269  | 0.893706  |
| 1 | -0.774547 | 1.443435  | 2.360908  |
| 1 | -0.069552 | 2.114200  | 1.027504  |
| 7 | 1.922540  | -2.839645 | 1.671433  |
| 1 | 2.681499  | -2.386700 | 2.173385  |
| 1 | 2.336071  | -3.613549 | 1.139880  |
| 1 | 1.324121  | -3.257205 | 2.379416  |
| 7 | -1.116216 | 0.025723  | -3.177802 |
| 1 | -0.860635 | 0.960675  | -2.849890 |
| 1 | -0.250516 | -0.504396 | -3.240711 |
| 1 | -1.474357 | 0.119343  | -4.124272 |
| 7 | 1.766265  | 0.816045  | -1.816602 |
| 1 | 2.517307  | 1.230179  | -1.264192 |
| 1 | 1.033527  | 1.525227  | -1.901585 |
| 1 | 2.140494  | 0.653535  | -2.747538 |
| 7 | -2.004894 | -2.261656 | -1.142244 |
| 1 | -1.964224 | -3.236291 | -1.424713 |
| 1 | -2.058621 | -1.691350 | -1.987264 |
| 1 | -2.867844 | -2.130188 | -0.612244 |
| 7 | 1.646694  | 3.609836  | 0.367777  |
| 1 | 1.837533  | 4.487993  | -0.108462 |
| 1 | 2.447640  | 3.001619  | 0.191084  |
| 1 | 1.644684  | 3.823215  | 1.361839  |
| 7 | -1.101507 | 1.778012  | 4.488873  |
| 1 | -1.686481 | 2.600230  | 4.605880  |
| 1 | -0.261063 | 1.933949  | 5.037382  |
| 1 | -1.593837 | 1.002371  | 4.921962  |
| 7 | 3.207615  | -5.280822 | 0.152050  |
| 1 | 3.924414  | -5.700773 | 0.736989  |
| 1 | 3.647479  | -5.055677 | -0.735404 |
| 1 | 2.522396  | -6.006757 | -0.036425 |
| 7 | -0.733424 | 2.783490  | -1.617623 |
| 1 | -0.092490 | 3.183731  | -0.928864 |
| 1 | -1.533428 | 2.413534  | -1.103493 |
| 1 | -1.070252 | 3.548489  | -2.195669 |
| 7 | 4.454609  | 2.045350  | -0.302445 |
| 1 | 4.863541  | 2.514373  | 0.501902  |
| 1 | 4.852661  | 2.490283  | -1.125664 |
| 1 | 4.809987  | 1.092836  | -0.286362 |

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Cartesian coordinates of : BDC13

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.338047 | 0.675392  | 0.013822  |
| 1  | -0.930821 | 1.277947  | -0.741201 |
| 1  | -0.667527 | 0.742326  | 0.817027  |
| 1  | -2.292051 | 0.997342  | 0.285488  |
| 1  | -1.465132 | -0.308135 | -0.305737 |
| 7  | -4.164114 | 1.039949  | 0.614686  |
| 1  | -4.679988 | 1.774989  | 0.138789  |
| 1  | -4.532841 | 0.151607  | 0.266355  |
| 1  | -4.417374 | 1.099759  | 1.597186  |
| 7  | 0.142061  | 2.414845  | -1.744935 |
| 1  | 0.354487  | 2.082337  | -2.681537 |
| 1  | -0.211250 | 3.362041  | -1.849603 |
| 1  | 1.031722  | 2.474008  | -1.233965 |
| 7  | -2.293706 | -1.966279 | -0.765089 |
| 1  | -2.024608 | -2.752068 | -0.179742 |
| 1  | -2.150535 | -2.258505 | -1.727735 |
| 1  | -3.299885 | -1.821753 | -0.637175 |
| 7  | -5.485049 | -1.728207 | -0.476148 |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | -5.630566  | -2.513935 | 0.153363  |
| 1 | -5.622223  | -2.092506 | -1.416110 |
| 1 | -6.259663  | -1.071299 | -0.306255 |
| 7 | 7.805206   | -1.832338 | 0.400553  |
| 1 | 7.557799   | -2.755822 | 0.056764  |
| 1 | 8.749414   | -1.628362 | 0.060609  |
| 1 | 7.862870   | -1.907928 | 1.412058  |
| 7 | 0.737354   | 1.230688  | 1.926201  |
| 1 | 0.585749   | 1.234419  | 2.930919  |
| 1 | 1.580926   | 0.676216  | 1.742537  |
| 1 | 0.959496   | 2.185418  | 1.653183  |
| 7 | 5.746767   | 0.317873  | -0.481664 |
| 1 | 6.444445   | -0.386519 | -0.206846 |
| 1 | 5.644595   | 0.249351  | -1.490578 |
| 1 | 6.160409   | 1.227228  | -0.293876 |
| 7 | 2.880707   | 2.435662  | -0.215188 |
| 1 | 3.057954   | 1.568223  | 0.293665  |
| 1 | 3.142712   | 3.200374  | 0.401703  |
| 1 | 3.552200   | 2.451073  | -0.978689 |
| 7 | -7.714666  | 0.341115  | 0.065356  |
| 1 | -7.773780  | 1.079885  | -0.630186 |
| 1 | -7.666940  | 0.800793  | 0.970480  |
| 1 | -8.607409  | -0.162693 | 0.036190  |
| 7 | 3.380314   | -0.418696 | 1.355717  |
| 1 | 3.768596   | -0.527283 | 2.289387  |
| 1 | 4.175361   | -0.228235 | 0.730093  |
| 1 | 3.014485   | -1.330182 | 1.092660  |
| 7 | -10.478779 | -1.181345 | -0.031595 |
| 1 | -10.609052 | -1.690614 | -0.900701 |
| 1 | -11.252061 | -0.527106 | 0.045352  |
| 1 | -10.585535 | -1.853389 | 0.722496  |
| 7 | 10.745639  | -1.232144 | -0.637968 |
| 1 | 11.343978  | -2.046551 | -0.537054 |
| 1 | 11.187290  | -0.474629 | -0.125680 |
| 1 | 10.758941  | -0.973426 | -1.619872 |

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Cartesian coordinates of : BC13\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.197956 | 0.350172  | 0.276947  |
| 1  | -0.393110 | -0.318938 | 1.050483  |
| 1  | 0.637752  | 0.032211  | -0.281281 |
| 1  | -1.056617 | 0.331901  | -0.309611 |
| 1  | -0.031235 | 1.315437  | 0.658406  |
| 7  | -2.814539 | -0.135515 | -0.965363 |
| 1  | -2.818315 | -0.609542 | -1.864312 |
| 1  | -3.207126 | -0.789264 | -0.283799 |
| 1  | -3.473117 | 0.634512  | -1.042898 |
| 7  | -1.264175 | -1.612393 | 2.171753  |
| 1  | -2.192298 | -1.765956 | 1.767054  |
| 1  | -0.792626 | -2.511930 | 2.200885  |
| 1  | -1.397795 | -1.321901 | 3.136139  |
| 7  | 0.286895  | 3.003789  | 1.321491  |
| 1  | 0.375785  | 3.693300  | 0.561226  |
| 1  | 1.148852  | 3.045226  | 1.859163  |
| 1  | -0.448878 | 3.338044  | 1.938330  |
| 7  | -4.226757 | -2.237533 | 1.087688  |
| 1  | -4.612298 | -2.144605 | 2.024536  |
| 1  | -4.115668 | -3.235951 | 0.927724  |
| 1  | -4.961276 | -1.918374 | 0.440639  |
| 7  | 0.560422  | 5.086871  | -0.933950 |
| 1  | -0.243981 | 5.116093  | -1.553992 |
| 1  | 0.662903  | 6.023914  | -0.532309 |
| 1  | 1.371724  | 4.927965  | -1.524704 |
| 7  | 2.098214  | -0.512934 | -1.223926 |
| 1  | 1.886174  | -1.200306 | -1.942491 |
| 1  | 2.564328  | 0.256601  | -1.697724 |
| 1  | 2.796912  | -0.942860 | -0.598169 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 9.095797  | -3.682313 | 0.221437  |
| 1 | 9.898388  | -3.800020 | -0.389600 |
| 1 | 9.409892  | -3.146621 | 1.024944  |
| 1 | 8.842773  | -4.605395 | 0.560728  |
| 7 | 4.225517  | -1.790078 | 0.568289  |
| 1 | 5.046379  | -1.944495 | -0.030749 |
| 1 | 3.972185  | -2.692410 | 0.960858  |
| 1 | 4.530864  | -1.215006 | 1.348363  |
| 7 | -6.346510 | -1.199391 | -0.909330 |
| 1 | -6.073320 | -1.248130 | -1.886909 |
| 1 | -6.638486 | -0.240914 | -0.739176 |
| 1 | -7.181412 | -1.785356 | -0.804838 |
| 7 | 6.686153  | -2.258192 | -1.284072 |
| 1 | 6.446808  | -2.845654 | -2.077638 |
| 1 | 7.456268  | -2.718457 | -0.790701 |
| 1 | 7.053316  | -1.392055 | -1.667600 |
| 7 | -8.932769 | -2.984791 | -0.589795 |
| 1 | -8.754489 | -3.968763 | -0.767657 |
| 1 | -9.659991 | -2.695085 | -1.237160 |
| 1 | -9.326936 | -2.920850 | 0.344124  |
| 7 | 0.895495  | 8.001354  | 0.262830  |
| 1 | 0.078598  | 8.314321  | 0.778808  |
| 1 | 1.050648  | 8.675042  | -0.481365 |
| 1 | 1.687908  | 8.070954  | 0.894285  |

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Cartesian coordinates of : BC13\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -3.587512 | 0.218501  | -0.097523 |
| 1  | -3.342405 | 0.008126  | 0.897401  |
| 1  | -3.337472 | 1.207393  | -0.331018 |
| 1  | -3.009759 | -0.447298 | -0.663208 |
| 1  | -4.607098 | 0.057266  | -0.268686 |
| 7  | -1.828879 | -1.797660 | -1.183004 |
| 1  | -0.868493 | -1.450103 | -1.281813 |
| 1  | -1.818073 | -2.439302 | -0.393281 |
| 1  | -2.043777 | -2.343984 | -2.012216 |
| 7  | -2.555293 | -0.676716 | 2.461755  |
| 1  | -2.250617 | 0.028553  | 3.127050  |
| 1  | -3.125027 | -1.336588 | 2.983976  |
| 1  | -1.716363 | -1.178388 | 2.145384  |
| 7  | -6.442563 | -0.181064 | -0.594602 |
| 1  | -7.012753 | 0.294570  | 0.099883  |
| 1  | -6.737187 | -1.164252 | -0.595596 |
| 1  | -6.711011 | 0.205556  | -1.495852 |
| 7  | -2.866764 | 2.973928  | -0.761822 |
| 1  | -2.912491 | 3.144938  | -1.762965 |
| 1  | -3.463669 | 3.677742  | -0.312675 |
| 1  | -1.910733 | 3.176789  | -0.481653 |
| 7  | -7.491816 | -3.141684 | -0.632298 |
| 1  | -8.471836 | -3.120778 | -0.899812 |
| 1  | -7.019290 | -3.744097 | -1.299878 |
| 1  | -7.444645 | -3.607924 | 0.268998  |
| 7  | -4.625925 | 5.215370  | 0.562059  |
| 1  | -4.100754 | 6.085178  | 0.559095  |
| 1  | -4.888891 | 5.035315  | 1.526566  |
| 1  | -5.486176 | 5.392617  | 0.051552  |
| 7  | 0.072779  | -2.059269 | 1.437198  |
| 1  | 0.420115  | -1.658948 | 0.564428  |
| 1  | 0.150797  | -3.069449 | 1.350270  |
| 1  | 0.744662  | -1.788376 | 2.150824  |
| 7  | 3.217356  | -0.512603 | 0.868388  |
| 1  | 4.025920  | -0.160733 | 0.336118  |
| 1  | 3.513029  | -1.386125 | 1.296401  |
| 1  | 3.062835  | 0.142922  | 1.629712  |
| 7  | 5.642942  | 0.491144  | -0.757802 |
| 1  | 5.714702  | 0.060282  | -1.675128 |
| 1  | 6.498537  | 0.249109  | -0.243653 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 5.662090  | 1.495411  | -0.910669 |
| 7 | 1.167905  | -0.806891 | -1.415439 |
| 1 | 1.061765  | 0.079447  | -1.902250 |
| 1 | 1.590481  | -1.446921 | -2.083397 |
| 1 | 1.866738  | -0.655069 | -0.674932 |
| 7 | 8.226846  | -0.249926 | 0.835831  |
| 1 | 8.257525  | 0.232087  | 1.729511  |
| 1 | 9.082320  | -0.004317 | 0.330321  |
| 1 | 8.275142  | -1.243504 | 1.041599  |
| 7 | 10.890667 | 0.508758  | -0.729645 |
| 1 | 11.720224 | 0.390734  | -0.155957 |
| 1 | 10.877299 | 1.475710  | -1.039355 |
| 1 | 11.016148 | -0.066801 | -1.556764 |

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Cartesian coordinates of : P\_NH3\_N13\_6.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.002697 | 0.434608  | -0.370792 |
| 1  | -0.622200 | -0.265985 | -0.849139 |
| 1  | 0.912840  | 0.479078  | -0.865968 |
| 1  | -0.543389 | 1.345497  | -0.405310 |
| 1  | 0.195344  | 0.117453  | 0.597246  |
| 7  | -1.821341 | 2.560204  | -0.695390 |
| 1  | -1.643141 | 3.163343  | -1.494131 |
| 1  | -2.647508 | 2.000330  | -0.925680 |
| 1  | -2.070757 | 3.173571  | 0.086888  |
| 7  | -2.001641 | -1.216996 | -1.576527 |
| 1  | -2.253593 | -1.898135 | -0.859574 |
| 1  | -2.738811 | -0.508040 | -1.573538 |
| 1  | -2.031162 | -1.681076 | -2.479660 |
| 7  | 1.106931  | -0.870391 | 2.002250  |
| 1  | 0.887361  | -0.982266 | 2.987428  |
| 1  | 2.071736  | -0.546603 | 1.932051  |
| 1  | 1.061943  | -1.787362 | 1.558175  |
| 7  | 2.655791  | 0.081780  | -1.544277 |
| 1  | 2.674718  | -0.155576 | -2.532559 |
| 1  | 3.368568  | 0.795434  | -1.392869 |
| 1  | 2.958698  | -0.744457 | -1.026224 |
| 7  | 3.793885  | 0.922423  | 1.414954  |
| 1  | 4.393994  | 1.099143  | 2.216717  |
| 1  | 4.289222  | 1.266213  | 0.589275  |
| 1  | 2.983182  | 1.527350  | 1.525998  |
| 7  | 5.226640  | 2.177452  | -1.241517 |
| 1  | 5.889442  | 2.673503  | -0.650323 |
| 1  | 4.779365  | 2.887553  | -1.816108 |
| 1  | 5.783654  | 1.604896  | -1.870961 |
| 7  | -4.512647 | 0.788003  | -1.166212 |
| 1  | -4.976181 | 1.531943  | -0.650273 |
| 1  | -4.728168 | -0.090252 | -0.678528 |
| 1  | -4.974358 | 0.748537  | -2.071444 |
| 7  | -4.813468 | -1.971997 | 0.244137  |
| 1  | -3.904040 | -2.256330 | 0.611772  |
| 1  | -5.125466 | -2.701534 | -0.390692 |
| 1  | -5.469750 | -1.965722 | 1.019755  |
| 7  | 3.799009  | -2.138652 | 0.486126  |
| 1  | 3.944722  | -1.227417 | 0.928294  |
| 1  | 4.662217  | -2.389168 | 0.010753  |
| 1  | 3.680654  | -2.818732 | 1.233334  |
| 7  | -1.787238 | -2.561344 | 1.278734  |
| 1  | -0.889646 | -2.725399 | 0.814943  |
| 1  | -1.946342 | -3.337606 | 1.915418  |
| 1  | -1.672937 | -1.728106 | 1.850965  |
| 7  | 0.840708  | -2.833560 | -0.518365 |
| 1  | 1.836526  | -2.620558 | -0.419457 |
| 1  | 0.471055  | -2.262487 | -1.275690 |
| 1  | 0.774719  | -3.800536 | -0.826070 |
| 7  | -2.644707 | 4.569985  | 1.620970  |

|   |           |          |          |
|---|-----------|----------|----------|
| 1 | -3.008455 | 4.139022 | 2.465756 |
| 1 | -3.374090 | 5.181575 | 1.265753 |
| 1 | -1.874555 | 5.168299 | 1.905033 |

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Cartesian coordinates of : P\_NH3\_N13\_13.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.700731  | -0.560878 | -0.348377 |
| 1  | -0.215424 | -0.653669 | -0.850037 |
| 1  | 0.454782  | -0.795390 | 0.629446  |
| 1  | 1.413221  | -1.224978 | -0.729502 |
| 1  | 1.055292  | 0.437423  | -0.384401 |
| 7  | -0.843724 | 1.691988  | -2.515525 |
| 1  | -0.885620 | 2.537901  | -3.077599 |
| 1  | -1.539863 | 1.046588  | -2.889690 |
| 1  | 0.069384  | 1.276482  | -2.681239 |
| 7  | -1.646025 | 1.886495  | 0.553191  |
| 1  | -2.235474 | 2.709883  | 0.649742  |
| 1  | -0.830337 | 2.035675  | 1.150922  |
| 1  | -1.319510 | 1.883263  | -0.419154 |
| 7  | -2.060600 | -0.850060 | -1.080224 |
| 1  | -2.366455 | -0.047507 | -0.528483 |
| 1  | -2.489677 | -0.770117 | -2.001160 |
| 1  | -2.406949 | -1.689354 | -0.617005 |
| 7  | 2.699731  | -2.394521 | -1.440882 |
| 1  | 2.288450  | -3.093021 | -2.054481 |
| 1  | 3.210341  | -2.904215 | -0.710717 |
| 1  | 3.394584  | -1.901539 | -1.995645 |
| 7  | 0.648324  | 1.602050  | 2.804887  |
| 1  | 1.298163  | 2.098958  | 3.408028  |
| 1  | -0.258724 | 1.587435  | 3.282154  |
| 1  | 0.963150  | 0.635779  | 2.759614  |
| 7  | -1.024122 | -0.963792 | 1.960788  |
| 1  | -1.464730 | -0.089361 | 1.665671  |
| 1  | -1.058097 | -0.986331 | 2.976167  |
| 1  | -1.603488 | -1.728890 | 1.611798  |
| 7  | 1.544959  | 2.148970  | -0.232675 |
| 1  | 2.490712  | 2.479061  | -0.446514 |
| 1  | 1.371760  | 2.290214  | 0.765100  |
| 1  | 0.889860  | 2.744216  | -0.734268 |
| 7  | -3.030787 | -3.401713 | 0.859033  |
| 1  | -2.738494 | -3.932322 | 1.675779  |
| 1  | -3.017523 | -4.055339 | 0.080350  |
| 1  | -4.004057 | -3.151214 | 1.012344  |
| 7  | -3.275038 | 0.010827  | -4.023516 |
| 1  | -3.963289 | 0.751895  | -3.918588 |
| 1  | -3.800710 | -0.850135 | -4.151607 |
| 1  | -2.794966 | 0.181523  | -4.903430 |
| 7  | 4.315319  | -3.996878 | 0.722367  |
| 1  | 4.881729  | -4.702529 | 0.260186  |
| 1  | 3.729882  | -4.484684 | 1.394032  |
| 1  | 4.952873  | -3.414585 | 1.257547  |
| 7  | -2.378459 | 1.556338  | 3.661799  |
| 1  | -2.852221 | 0.872201  | 4.244414  |
| 1  | -2.764582 | 1.479208  | 2.722873  |
| 1  | -2.636729 | 2.470646  | 4.022590  |
| 7  | 4.422805  | 3.333457  | -0.874192 |
| 1  | 4.685277  | 3.326699  | -1.855401 |
| 1  | 5.180078  | 2.887823  | -0.364652 |
| 1  | 4.405575  | 4.306336  | -0.581910 |

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Cartesian coordinates of : P\_NH3\_N13\_15.log

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 0.279183  | 0.223382  | 0.038012  |
| 1 | -0.231565 | 0.977811  | -0.469931 |
| 1 | 0.941281  | 0.635146  | 0.760328  |
| 1 | -0.472715 | -0.333330 | 0.502348  |
| 1 | 0.806418  | -0.365101 | -0.638384 |
| 7 | -2.195548 | -0.847584 | 1.110287  |
| 1 | -2.409342 | -0.407593 | 2.001925  |
| 1 | -2.818832 | -0.419608 | 0.420799  |
| 1 | -2.480190 | -1.823435 | 1.198640  |
| 7 | -1.625103 | 2.061716  | -1.191487 |
| 1 | -2.479835 | 1.498519  | -1.105034 |
| 1 | -1.780179 | 2.922220  | -0.673609 |
| 1 | -1.537412 | 2.325528  | -2.168880 |
| 7 | 1.662200  | -1.409506 | -2.034956 |
| 1 | 1.212620  | -2.315228 | -2.142334 |
| 1 | 2.672367  | -1.586519 | -1.988379 |
| 1 | 1.496784  | -0.908507 | -2.904504 |
| 7 | -4.272487 | 0.366215  | -1.125611 |
| 1 | -4.228924 | -0.066649 | -2.045147 |
| 1 | -4.863672 | 1.196503  | -1.225617 |
| 1 | -4.773336 | -0.295063 | -0.523791 |
| 7 | -6.119018 | 2.956603  | -1.520626 |
| 1 | -7.011463 | 2.626195  | -1.875873 |
| 1 | -6.310834 | 3.450272  | -0.654122 |
| 1 | -5.774286 | 3.644415  | -2.183445 |
| 7 | 2.136316  | 1.212477  | 1.928763  |
| 1 | 2.404579  | 2.197895  | 1.859541  |
| 1 | 1.894149  | 1.043078  | 2.901197  |
| 1 | 2.952623  | 0.630557  | 1.715620  |
| 7 | -3.074255 | -4.001777 | 1.669729  |
| 1 | -2.102360 | -4.160144 | 1.922724  |
| 1 | -3.630407 | -4.316541 | 2.460522  |
| 1 | -3.278144 | -4.633804 | 0.900041  |
| 7 | 4.148047  | -0.988255 | 0.983681  |
| 1 | 4.353312  | -1.670827 | 1.707378  |
| 1 | 5.026256  | -0.757922 | 0.521833  |
| 1 | 3.577696  | -1.452367 | 0.280885  |
| 7 | -5.431864 | -1.802086 | 0.868816  |
| 1 | -5.759474 | -1.367772 | 1.726566  |
| 1 | -4.673816 | -2.435737 | 1.118643  |
| 1 | -6.199477 | -2.361821 | 0.509701  |
| 7 | 4.729651  | -2.082793 | -1.992417 |
| 1 | 4.945123  | -2.974729 | -1.554482 |
| 1 | 5.378509  | -1.399420 | -1.597795 |
| 1 | 4.960936  | -2.185075 | -2.977024 |
| 7 | 6.855836  | 0.027416  | -0.652554 |
| 1 | 7.405906  | 0.072629  | -1.506498 |
| 1 | 7.499375  | -0.247187 | 0.085115  |
| 1 | 6.563190  | 0.979044  | -0.447070 |
| 7 | 2.882277  | 4.316967  | 1.940538  |
| 1 | 3.066170  | 4.755095  | 1.043073  |
| 1 | 3.706612  | 4.462071  | 2.515951  |
| 1 | 2.125708  | 4.837969  | 2.373855  |

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Cartesian coordinates of : P\_NH3\_N13\_10.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y        | Z         |
|----|-----------|----------|-----------|
| 7  | -0.001076 | 2.002686 | 0.522965  |
| 1  | -0.002479 | 3.011998 | 0.829987  |
| 1  | -0.880108 | 1.783657 | -0.044682 |
| 1  | 0.878761  | 1.785656 | -0.044249 |
| 1  | -0.000617 | 1.411443 | 1.352187  |
| 7  | 2.340077  | 1.364192 | -0.890764 |
| 1  | 2.918320  | 2.163564 | -1.137172 |
| 1  | 2.913742  | 0.753995 | -0.282948 |
| 1  | 2.180258  | 0.852652 | -1.755069 |
| 7  | -0.006657 | 4.738145 | 1.412302  |
| 1  | 0.799100  | 4.947939 | 1.996258  |

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|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | 0.004629   | 5.414361  | 0.638906  |
| 1 | -0.827117  | 4.950194  | 1.974575  |
| 7 | 10.955841  | -3.861793 | -0.592242 |
| 1 | 11.668505  | -4.225926 | 0.032855  |
| 1 | 11.399501  | -3.155130 | -1.170958 |
| 1 | 10.683015  | -4.621928 | -1.207770 |
| 7 | 4.021207   | -0.427592 | 0.870278  |
| 1 | 3.588066   | -1.297891 | 1.166943  |
| 1 | 4.401248   | 0.000519  | 1.710143  |
| 1 | 4.824908   | -0.683768 | 0.279331  |
| 7 | -10.965402 | -3.847451 | -0.593603 |
| 1 | -10.693066 | -4.607428 | -1.209543 |
| 1 | -11.678365 | -4.211434 | 0.031241  |
| 1 | -11.408531 | -3.140153 | -1.171950 |
| 7 | -2.340351  | 1.359414  | -0.891983 |
| 1 | -2.919906  | 2.157564  | -1.139287 |
| 1 | -2.179093  | 0.847593  | -1.755856 |
| 1 | -2.913389  | 0.748610  | -0.284177 |
| 7 | -8.480509  | -2.648726 | 0.989839  |
| 1 | -9.276866  | -3.037138 | 0.477321  |
| 1 | -8.043269  | -3.416213 | 1.491538  |
| 1 | -8.855568  | -2.019828 | 1.693941  |
| 7 | -4.020432  | -0.433775 | 0.868531  |
| 1 | -4.824932  | -0.688148 | 0.277892  |
| 1 | -4.399273  | -0.007008 | 1.709619  |
| 1 | -3.587636  | -1.304977 | 1.163039  |
| 7 | 6.438189   | -1.207679 | -0.883441 |
| 1 | 6.923486   | -0.423348 | -1.309568 |
| 1 | 6.210197   | -1.847916 | -1.638753 |
| 1 | 7.115236   | -1.686852 | -0.277501 |
| 7 | -6.439608  | -1.208071 | -0.884719 |
| 1 | -6.921586  | -0.422895 | -1.313050 |
| 1 | -7.118992  | -1.683298 | -0.278285 |
| 1 | -6.213425  | -1.850896 | -1.638377 |
| 7 | 8.471801   | -2.659903 | 0.990118  |
| 1 | 8.847522   | -2.033820 | 1.696374  |
| 1 | 9.267869   | -3.049393 | 0.477969  |
| 1 | 8.031481   | -3.427330 | 1.489210  |
| 7 | 0.026555   | 6.897340  | -0.848324 |
| 1 | 0.885624   | 6.912743  | -1.390447 |
| 1 | -0.057043  | 7.809784  | -0.408839 |
| 1 | -0.737665  | 6.822945  | -1.513548 |

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Cartesian coordinates of the protonated ammonia tetradecamer

Cartesian coordinates of : Ca14

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.295644  | -1.437114 | 2.010243  |
| 1  | 0.230112  | 0.321249  | 2.468985  |
| 1  | 1.287223  | -1.910726 | 2.910622  |
| 1  | 0.950501  | -2.114362 | 1.327574  |
| 1  | 2.271792  | -1.255246 | 1.778641  |
| 7  | -2.016734 | -1.825500 | 1.463488  |
| 1  | -2.299877 | -2.288395 | 2.324224  |
| 1  | -1.542279 | -0.967347 | 1.743127  |
| 1  | -1.293870 | -2.415132 | 1.039213  |
| 7  | -1.983867 | 1.309875  | 0.045469  |
| 1  | -2.949638 | 0.931521  | 0.143945  |
| 1  | -1.991986 | 2.289460  | -0.340688 |
| 1  | -1.423105 | 0.663105  | -0.563905 |
| 7  | -0.346300 | 1.170567  | 2.488152  |
| 1  | -1.517928 | 1.315611  | 0.976975  |
| 1  | -0.717628 | 1.282178  | 3.427397  |
| 1  | 0.283061  | 1.952418  | 2.319008  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 0.104470  | -3.513008 | -0.241345 |
| 1 | -0.591653 | -3.484095 | -0.986627 |
| 1 | 0.220898  | -4.486093 | 0.027326  |
| 1 | 0.992192  | -3.192624 | -0.637806 |
| 7 | -2.769239 | -2.620429 | -1.562728 |
| 1 | -3.397064 | -2.056672 | -2.129087 |
| 1 | -2.847363 | -2.305988 | -0.594314 |
| 1 | -3.119718 | -3.573280 | -1.607794 |
| 7 | -4.501989 | -0.103358 | 0.526687  |
| 1 | -3.986351 | -0.913854 | 0.874944  |
| 1 | -5.124799 | -0.415910 | -0.212209 |
| 1 | -5.092344 | 0.240140  | 1.278882  |
| 7 | -0.396930 | -0.621998 | -1.396842 |
| 1 | 0.167194  | -1.150658 | -0.731604 |
| 1 | 0.253043  | -0.296721 | -2.111264 |
| 1 | -1.028636 | -1.307992 | -1.815943 |
| 7 | 2.689433  | -1.844248 | -1.062697 |
| 1 | 3.330752  | -2.487010 | -1.520285 |
| 1 | 3.198606  | -1.408879 | -0.293721 |
| 1 | 2.473966  | -1.106364 | -1.732630 |
| 7 | 4.483019  | -0.523057 | 1.458450  |
| 1 | 4.869725  | -1.416055 | 1.756221  |
| 1 | 4.442357  | 0.059252  | 2.292048  |
| 1 | 5.184570  | -0.101520 | 0.854013  |
| 7 | 2.073112  | 0.660053  | -3.278173 |
| 1 | 3.053150  | 0.933428  | -3.276678 |
| 1 | 1.544927  | 1.504731  | -3.485471 |
| 1 | 1.953604  | 0.046690  | -4.081329 |
| 7 | -1.823172 | 4.037429  | -0.822078 |
| 1 | -0.876772 | 4.262513  | -0.488545 |
| 1 | -2.472109 | 4.668879  | -0.360521 |
| 1 | -1.864813 | 4.256155  | -1.813352 |
| 7 | 1.046479  | 4.252379  | 0.279688  |
| 1 | 1.383691  | 3.285527  | 0.295490  |
| 1 | 1.126816  | 4.630401  | 1.219291  |
| 1 | 1.686850  | 4.790598  | -0.297049 |
| 7 | 1.807619  | 1.175961  | 0.096097  |
| 1 | 1.079614  | 0.549384  | 0.434544  |
| 1 | 2.678802  | 0.803829  | 0.472072  |
| 1 | 1.843686  | 1.044980  | -0.914594 |

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Cartesian coordinates of : BDC14\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.236669  | -0.293693 | 0.478860  |
| 1  | -0.365055 | -1.081613 | 0.167254  |
| 1  | -0.436127 | 0.474600  | 0.751216  |
| 1  | 0.858925  | -0.569623 | 1.279356  |
| 1  | 0.883783  | 0.009738  | -0.275479 |
| 7  | 2.313164  | -0.878743 | 2.367073  |
| 1  | 2.393503  | -0.212771 | 3.130536  |
| 1  | 2.382930  | -1.813890 | 2.778786  |
| 1  | 3.125531  | -0.739412 | 1.762583  |
| 7  | -1.958271 | -2.092481 | -0.267635 |
| 1  | -2.146050 | -2.876415 | 0.351038  |
| 1  | -2.730850 | -1.429260 | -0.153547 |
| 1  | -2.019107 | -2.451625 | -1.216281 |
| 7  | 2.528838  | 0.418701  | -1.211630 |
| 1  | 3.280203  | 0.123563  | -0.581483 |
| 1  | 2.668097  | 1.408112  | -1.396671 |
| 1  | 2.679532  | -0.064299 | -2.092846 |
| 7  | 6.189623  | 0.150397  | -2.230976 |
| 1  | 5.853672  | 1.035865  | -2.599075 |
| 1  | 5.977124  | -0.553273 | -2.932615 |
| 1  | 7.210871  | 0.217215  | -2.177186 |
| 7  | 5.035176  | -0.514332 | 0.566326  |
| 1  | 5.290790  | -1.470206 | 0.801334  |
| 1  | 5.475136  | -0.306589 | -0.340354 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 5.490583  | 0.079276  | 1.255070  |
| 7 | -1.899285 | 1.468464  | 1.097518  |
| 1 | -2.683715 | 0.906570  | 0.761353  |
| 1 | -2.064412 | 1.651093  | 2.083460  |
| 1 | -1.932347 | 2.374964  | 0.614700  |
| 7 | -4.505404 | -0.163904 | -0.086950 |
| 1 | -4.904728 | -0.963576 | -0.596284 |
| 1 | -5.065440 | -0.041852 | 0.752915  |
| 1 | -4.668536 | 0.659782  | -0.660741 |
| 7 | -5.528764 | -2.660782 | -1.615604 |
| 1 | -5.216415 | -2.694382 | -2.581988 |
| 1 | -6.553250 | -2.673674 | -1.633995 |
| 1 | -5.229280 | -3.530848 | -1.184676 |
| 7 | -8.693492 | -2.712529 | -1.703718 |
| 1 | -9.110402 | -2.787265 | -0.780662 |
| 1 | -9.035325 | -3.499458 | -2.247355 |
| 1 | -9.069939 | -1.871605 | -2.131035 |
| 7 | 9.344807  | 0.336612  | -2.075804 |
| 1 | 9.661107  | 1.116948  | -1.507897 |
| 1 | 9.760446  | 0.452456  | -2.995292 |
| 1 | 9.747312  | -0.504352 | -1.672950 |
| 7 | -1.967626 | 4.242530  | -0.333002 |
| 1 | -2.502301 | 4.929669  | 0.205901  |
| 1 | -2.367836 | 4.218567  | -1.266473 |
| 1 | -1.026525 | 4.611907  | -0.433395 |
| 7 | 2.505243  | -3.733206 | 3.755871  |
| 1 | 3.316448  | -3.793586 | 4.364101  |
| 1 | 2.558993  | -4.517009 | 3.112333  |
| 1 | 1.687771  | -3.885243 | 4.339176  |
| 7 | -3.582291 | 6.429009  | 1.318567  |
| 1 | -4.542026 | 6.158882  | 1.511383  |
| 1 | -3.617951 | 7.307245  | 0.809673  |
| 1 | -3.143845 | 6.623072  | 2.213836  |

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Cartesian coordinates of : BC14

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.732713  | 0.057103  | 0.013543  |
| 1  | 0.049964  | -0.424945 | 0.658336  |
| 1  | 1.169141  | -0.631624 | -0.643041 |
| 1  | 0.155900  | 0.742718  | -0.512649 |
| 1  | 1.478368  | 0.545960  | 0.562735  |
| 7  | -1.400285 | 1.734262  | -1.121834 |
| 1  | -1.579131 | 1.737158  | -2.122059 |
| 1  | -2.198941 | 1.268248  | -0.680938 |
| 1  | -1.418661 | 2.704835  | -0.821545 |
| 7  | -1.427550 | -0.976551 | 1.555205  |
| 1  | -2.207560 | -0.513201 | 1.085299  |
| 1  | -1.597058 | -1.989330 | 1.525326  |
| 1  | -1.461538 | -0.699187 | 2.532214  |
| 7  | 2.841950  | 1.372234  | 1.536978  |
| 1  | 2.959952  | 2.363734  | 1.287048  |
| 1  | 3.734976  | 0.916014  | 1.370091  |
| 1  | 2.686114  | 1.336169  | 2.540825  |
| 7  | -4.040636 | 0.343194  | 0.039802  |
| 1  | -4.499961 | 0.615540  | 0.905069  |
| 1  | -4.337046 | -0.610278 | -0.153001 |
| 1  | -4.435081 | 0.933311  | -0.704712 |
| 7  | 3.212599  | 4.353640  | 0.803570  |
| 1  | 2.371609  | 4.901663  | 0.960583  |
| 1  | 3.954794  | 4.776587  | 1.368825  |
| 1  | 3.466303  | 4.489060  | -0.170889 |
| 7  | 1.965356  | -1.862496 | -1.806589 |
| 1  | 1.573586  | -2.793622 | -1.693350 |
| 1  | 1.842128  | -1.618163 | -2.785559 |
| 1  | 2.978346  | -1.940672 | -1.643030 |
| 7  | -1.886424 | -4.069253 | 1.522611  |
| 1  | -2.406351 | -4.374869 | 2.350101  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -2.387380 | -4.418194 | 0.710605  |
| 1 | -0.992837 | -4.552435 | 1.539322  |
| 7 | 5.019042  | -2.117797 | -1.356797 |
| 1 | 5.401958  | -2.787314 | -2.031124 |
| 1 | 5.269549  | -2.453021 | -0.430979 |
| 1 | 5.517678  | -1.243014 | -1.492478 |
| 7 | -5.029281 | 2.195713  | -2.243221 |
| 1 | -4.811583 | 1.849437  | -3.173410 |
| 1 | -4.625061 | 3.125714  | -2.178849 |
| 1 | -6.046849 | 2.308313  | -2.198964 |
| 7 | 6.237316  | -4.176124 | -3.437308 |
| 1 | 5.849036  | -5.108965 | -3.334964 |
| 1 | 7.242894  | -4.259955 | -3.321388 |
| 1 | 6.073045  | -3.891402 | -4.398256 |
| 7 | 5.493422  | 5.701960  | 2.548205  |
| 1 | 5.608104  | 6.681286  | 2.304540  |
| 1 | 6.397690  | 5.257565  | 2.420876  |
| 1 | 5.283886  | 5.666636  | 3.541330  |
| 7 | -3.465769 | -5.090360 | 4.087806  |
| 1 | -4.381379 | -4.663802 | 4.192465  |
| 1 | -2.954386 | -4.907971 | 4.946047  |
| 1 | -3.610583 | -6.094367 | 4.036993  |
| 7 | -8.175051 | 2.538194  | -2.136642 |
| 1 | -8.524024 | 3.027648  | -2.955345 |
| 1 | -8.484326 | 3.063202  | -1.324123 |
| 1 | -8.647091 | 1.639498  | -2.105281 |

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Cartesian coordinates of : P\_NH3\_N14\_6.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.525201  | 0.795498  | -0.300685 |
| 1  | -0.098365 | 0.481977  | -1.091064 |
| 1  | 1.478333  | 1.054277  | -0.674346 |
| 1  | 0.028748  | 1.591532  | 0.152794  |
| 1  | 0.636054  | 0.008686  | 0.368900  |
| 7  | -1.441256 | 2.733947  | 0.604345  |
| 1  | -1.294263 | 3.738315  | 0.645096  |
| 1  | -2.088461 | 2.538865  | -0.162467 |
| 1  | -1.940043 | 2.461467  | 1.449923  |
| 7  | -1.397456 | 0.014357  | -2.281386 |
| 1  | -1.630939 | -0.972507 | -2.134007 |
| 1  | -2.214259 | 0.565719  | -2.004373 |
| 1  | -1.269209 | 0.157587  | -3.279495 |
| 7  | 0.974696  | -1.657978 | 1.289121  |
| 1  | 0.320930  | -2.266466 | 1.775245  |
| 1  | 1.832182  | -1.623381 | 1.840994  |
| 1  | 1.197264  | -2.104197 | 0.397118  |
| 7  | 3.161415  | 1.154211  | -1.323609 |
| 1  | 3.232608  | 1.077541  | -2.335198 |
| 1  | 3.666120  | 2.007229  | -1.059029 |
| 1  | 3.656821  | 0.352494  | -0.930369 |
| 7  | 3.620034  | -1.593594 | 3.269039  |
| 1  | 3.588668  | -2.556340 | 3.595388  |
| 1  | 4.580398  | -1.283018 | 3.394439  |
| 1  | 3.061908  | -1.048143 | 3.921171  |
| 7  | 4.703353  | 3.832971  | -0.712498 |
| 1  | 4.726344  | 4.140924  | 0.255176  |
| 1  | 4.276864  | 4.583637  | -1.248108 |
| 1  | 5.668760  | 3.765926  | -1.021955 |
| 7  | -3.926768 | 1.389182  | -0.819948 |
| 1  | -4.111681 | 1.587058  | 0.163364  |
| 1  | -4.255272 | 0.428493  | -0.984254 |
| 1  | -4.516262 | 2.012333  | -1.365454 |
| 7  | -4.357080 | -1.634012 | -0.881846 |
| 1  | -3.683209 | -2.109268 | -1.478362 |
| 1  | -5.249119 | -2.108978 | -0.977838 |
| 1  | -4.023605 | -1.762356 | 0.071806  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 4.202607  | -1.644089 | 0.030186  |
| 1 | 3.952018  | -1.521443 | 1.012946  |
| 1 | 5.193997  | -1.431884 | -0.051461 |
| 1 | 4.114786  | -2.638978 | -0.164667 |
| 7 | -1.413919 | -2.778640 | -0.984792 |
| 1 | -0.401508 | -2.702344 | -1.084204 |
| 1 | -1.652406 | -3.765914 | -0.977476 |
| 1 | -1.675484 | -2.382986 | -0.080739 |
| 7 | 1.577504  | -1.854600 | -1.804951 |
| 1 | 2.463978  | -1.484717 | -1.458022 |
| 1 | 1.091746  | -1.103074 | -2.290216 |
| 1 | 1.799496  | -2.557510 | -2.505193 |
| 7 | -4.185378 | 1.727572  | 2.586088  |
| 1 | -3.815470 | 1.658503  | 3.531125  |
| 1 | -5.010876 | 1.132945  | 2.562181  |
| 1 | -4.520650 | 2.682526  | 2.483148  |
| 7 | -2.179993 | -0.509438 | 1.098116  |
| 1 | -1.255224 | -0.473674 | 1.522088  |
| 1 | -2.790509 | 0.089799  | 1.654257  |
| 1 | -2.111913 | -0.048364 | 0.190866  |

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Cartesian coordinates of : P\_NH3\_N14\_7.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.316957  | 0.226242  | -0.311871 |
| 1  | 0.258427  | 0.111841  | -0.402486 |
| 1  | 1.619009  | -0.466207 | 0.400110  |
| 1  | 1.787177  | 0.041339  | -1.223145 |
| 1  | 1.533677  | 1.197492  | 0.007779  |
| 7  | -0.622469 | 4.931954  | -0.104779 |
| 1  | -0.860712 | 5.586928  | 0.635333  |
| 1  | -1.487451 | 4.710753  | -0.590970 |
| 1  | -0.046208 | 5.443717  | -0.767874 |
| 7  | -1.148005 | 2.269336  | 1.861971  |
| 1  | -1.716690 | 2.728794  | 2.568554  |
| 1  | -0.245478 | 2.060834  | 2.292745  |
| 1  | -0.970677 | 2.963204  | 1.136341  |
| 7  | -1.460230 | -0.120759 | -0.268872 |
| 1  | -1.734045 | 0.635023  | 0.361218  |
| 1  | -2.052995 | -0.086357 | -1.105725 |
| 1  | -1.646631 | -1.001500 | 0.209194  |
| 7  | 2.605781  | -0.229694 | -2.934226 |
| 1  | 2.384930  | -1.137966 | -3.333316 |
| 1  | 3.627968  | -0.144902 | -2.930288 |
| 1  | 2.255959  | 0.461799  | -3.592283 |
| 7  | 1.513254  | 1.006017  | 3.245296  |
| 1  | 0.769810  | 0.304663  | 3.294923  |
| 1  | 2.328907  | 0.534650  | 2.861976  |
| 1  | 1.747036  | 1.274252  | 4.197202  |
| 7  | 1.571137  | -1.904053 | 1.727409  |
| 1  | 1.333479  | -2.767632 | 1.239188  |
| 1  | 0.749206  | -1.635053 | 2.274200  |
| 1  | 2.312608  | -2.130626 | 2.384560  |
| 7  | 1.825396  | 2.917840  | 0.709892  |
| 1  | 2.706072  | 3.390988  | 0.531823  |
| 1  | 1.784514  | 2.692783  | 1.704620  |
| 1  | 1.073060  | 3.574836  | 0.497399  |
| 7  | -1.644685 | -3.243144 | 0.997459  |
| 1  | -2.003944 | -3.868889 | 1.713991  |
| 1  | -0.737416 | -3.614209 | 0.711952  |
| 1  | -2.270874 | -3.333537 | 0.201578  |
| 7  | -3.263544 | -0.073736 | -2.846885 |
| 1  | -3.115080 | 0.773367  | -3.387898 |
| 1  | -4.259391 | -0.106108 | -2.610854 |
| 1  | -3.082521 | -0.849335 | -3.477684 |
| 7  | 5.742980  | 0.052777  | -3.045155 |
| 1  | 6.066331  | -0.175760 | -3.980807 |
| 1  | 6.248587  | -0.551306 | -2.403947 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 6.047103  | 1.002998  | -2.854168 |
| 7 | -1.133650 | -0.750780 | 2.950620  |
| 1 | -1.471765 | -1.517581 | 2.364587  |
| 1 | -1.459479 | 0.119002  | 2.527324  |
| 1 | -1.589184 | -0.838824 | 3.854758  |
| 7 | 1.127367  | -4.848089 | 0.257271  |
| 1 | 0.570882  | -5.435727 | -0.358435 |
| 1 | 1.365627  | -5.421530 | 1.062495  |
| 1 | 1.997093  | -4.663377 | -0.235899 |
| 7 | -6.371635 | -0.149283 | -2.167658 |
| 1 | -6.811713 | -1.021166 | -2.446303 |
| 1 | -6.865017 | 0.596128  | -2.649892 |
| 1 | -6.550757 | -0.030211 | -1.175192 |

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Cartesian coordinates of : P\_NH3\_N14\_15.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.150264  | -0.040599 | 0.073214  |
| 1  | 0.574162  | 0.786553  | 0.546980  |
| 1  | -0.610588 | 0.251924  | -0.593447 |
| 1  | 0.945817  | -0.481513 | -0.444608 |
| 1  | -0.237740 | -0.701373 | 0.782685  |
| 7  | 2.661632  | -0.775720 | -1.152189 |
| 1  | 2.773768  | -0.330034 | -2.059369 |
| 1  | 3.269031  | -0.268564 | -0.503363 |
| 1  | 3.049817  | -1.714960 | -1.245671 |
| 7  | 1.850891  | 2.042478  | 1.199104  |
| 1  | 2.761911  | 1.587037  | 1.063305  |
| 1  | 1.882423  | 2.925660  | 0.697417  |
| 1  | 1.776979  | 2.274859  | 2.185717  |
| 7  | -0.891377 | -1.875855 | 2.126468  |
| 1  | -0.646253 | -2.848750 | 1.960985  |
| 1  | -1.907660 | -1.848049 | 2.280137  |
| 1  | -0.457625 | -1.624830 | 3.011515  |
| 7  | 4.678736  | 0.688594  | 0.984132  |
| 1  | 4.733198  | 0.252745  | 1.901739  |
| 1  | 5.170032  | 1.583980  | 1.061638  |
| 1  | 5.226509  | 0.093139  | 0.354979  |
| 7  | 6.236599  | 3.468740  | 1.321857  |
| 1  | 7.145937  | 3.235666  | 1.710036  |
| 1  | 6.405513  | 3.942982  | 0.439826  |
| 1  | 5.814701  | 4.148452  | 1.947378  |
| 7  | -2.022120 | 0.578389  | -1.704829 |
| 1  | -2.495322 | 1.479240  | -1.621974 |
| 1  | -1.820435 | 0.445230  | -2.692215 |
| 1  | -2.685118 | -0.154828 | -1.428313 |
| 7  | 3.867559  | -3.818687 | -1.687402 |
| 1  | 2.917414  | -4.101041 | -1.913759 |
| 1  | 4.445288  | -4.107360 | -2.472710 |
| 1  | 4.153870  | -4.383551 | -0.892112 |
| 7  | -3.850043 | -1.664215 | -0.547269 |
| 1  | -4.303591 | -2.429831 | -1.037912 |
| 1  | -4.561252 | -1.187505 | 0.009077  |
| 1  | -3.207842 | -2.080597 | 0.122899  |
| 7  | 5.988017  | -1.334056 | -1.068497 |
| 1  | 6.213677  | -0.875388 | -1.946258 |
| 1  | 5.301295  | -2.059046 | -1.271761 |
| 1  | 6.836588  | -1.791035 | -0.748113 |
| 7  | -3.960657 | -1.922577 | 2.683598  |
| 1  | -4.383180 | -2.832575 | 2.517513  |
| 1  | -4.565961 | -1.232622 | 2.229442  |
| 1  | -4.025254 | -1.761715 | 3.685512  |
| 7  | -5.930170 | 0.150606  | 1.209553  |
| 1  | -6.872314 | -0.209837 | 1.335995  |
| 1  | -5.883334 | 0.548091  | 0.264130  |
| 1  | -5.830891 | 0.922714  | 1.863317  |
| 7  | -3.444234 | 3.563318  | -1.660912 |
| 1  | -4.057414 | 3.873390  | -0.911616 |

|   |           |          |           |
|---|-----------|----------|-----------|
| 1 | -3.796251 | 3.978945 | -2.519298 |
| 1 | -2.537699 | 3.989045 | -1.487030 |
| 7 | -5.424294 | 0.919958 | -1.757146 |
| 1 | -6.183011 | 1.105680 | -2.406326 |
| 1 | -4.962243 | 0.065850 | -2.060031 |
| 1 | -4.742577 | 1.671198 | -1.854109 |

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Cartesian coordinates of : P\_NH3\_N14\_16.log

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Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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|   |            |           |           |
|---|------------|-----------|-----------|
| 7 | -0.473239  | 0.634596  | 0.197295  |
| 1 | -0.115761  | 1.207596  | -0.603843 |
| 1 | 0.231858   | 0.751567  | 0.963339  |
| 1 | -1.421049  | 0.949476  | 0.499650  |
| 1 | -0.592813  | -0.366103 | -0.069871 |
| 7 | -3.268124  | 0.951044  | 0.923529  |
| 1 | -3.844908  | 1.653806  | 0.469036  |
| 1 | -3.619360  | 0.046322  | 0.601226  |
| 1 | -3.473162  | 1.010654  | 1.917319  |
| 7 | 0.886566   | 2.310668  | -1.717911 |
| 1 | 1.047297   | 1.940581  | -2.650667 |
| 1 | 0.517639   | 3.249661  | -1.840591 |
| 1 | 1.803381   | 2.397815  | -1.262110 |
| 7 | -1.384500  | -2.062343 | -0.418224 |
| 1 | -1.104185  | -2.800895 | 0.220968  |
| 1 | -1.229245  | -2.417252 | -1.357681 |
| 1 | -2.394975  | -1.930249 | -0.306349 |
| 7 | -4.567302  | -1.820471 | -0.195553 |
| 1 | -4.799313  | -2.535847 | 0.489442  |
| 1 | -4.683771  | -2.257810 | -1.106761 |
| 1 | -5.302217  | -1.101887 | -0.126732 |
| 7 | 8.771533   | -1.660115 | 0.414666  |
| 1 | 8.503987   | -2.624353 | 0.238996  |
| 1 | 9.678002   | -1.512313 | -0.038209 |
| 1 | 8.922996   | -1.581459 | 1.416202  |
| 7 | 1.683140   | 1.306868  | 1.986394  |
| 1 | 1.580681   | 1.347483  | 2.996489  |
| 1 | 2.523394   | 0.754755  | 1.782434  |
| 1 | 1.878559   | 2.253023  | 1.667320  |
| 7 | 6.613226   | 0.336021  | -0.586429 |
| 1 | 7.342993   | -0.318587 | -0.274713 |
| 1 | 6.491363   | 0.184521  | -1.584023 |
| 1 | 6.995611   | 1.271845  | -0.480490 |
| 7 | 3.702157   | 2.413600  | -0.338666 |
| 1 | 3.905628   | 1.578939  | 0.213436  |
| 1 | 3.987801   | 3.214840  | 0.218421  |
| 1 | 4.338912   | 2.383432  | -1.130926 |
| 7 | -6.719647  | 0.370958  | 0.063829  |
| 1 | -6.762217  | 1.078644  | -0.664500 |
| 1 | -6.784155  | 0.864959  | 0.949732  |
| 1 | -7.574639  | -0.194797 | -0.023145 |
| 7 | 4.307326   | -0.349484 | 1.345359  |
| 1 | 4.723678   | -0.437912 | 2.268998  |
| 1 | 5.083145   | -0.173505 | 0.691933  |
| 1 | 3.933435   | -1.266164 | 1.113515  |
| 7 | -9.246060  | -1.409588 | -0.203865 |
| 1 | -9.197225  | -2.009859 | -1.022111 |
| 1 | -10.104592 | -0.857573 | -0.287483 |
| 1 | -9.364521  | -2.023995 | 0.596601  |
| 7 | 11.600839  | -1.226525 | -0.961636 |
| 1 | 12.260835  | -1.943877 | -0.676576 |
| 1 | 12.011257  | -0.330849 | -0.715428 |
| 1 | 11.545898  | -1.259121 | -1.975117 |
| 7 | -11.931409 | 0.265327  | -0.459182 |
| 1 | -12.742368 | -0.345916 | -0.473391 |
| 1 | -11.962723 | 0.819601  | -1.309525 |
| 1 | -12.056692 | 0.906914  | 0.317951  |

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Cartesian coordinates of : P\_NH3\_N14\_10.log

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | -0.018736  | 1.358060  | 0.569261  |
| 1  | -0.022540  | 2.375151  | 0.868668  |
| 1  | -0.891510  | 1.136227  | -0.002498 |
| 1  | 0.862833   | 1.138495  | 0.010009  |
| 1  | -0.024162  | 0.772555  | 1.402326  |
| 7  | 2.338842   | 0.722153  | -0.834493 |
| 1  | 2.916315   | 1.529155  | -1.056494 |
| 1  | 2.908551   | 0.098634  | -0.237607 |
| 1  | 2.186120   | 0.231866  | -1.712179 |
| 7  | -0.031425  | 4.086530  | 1.387910  |
| 1  | 0.704948   | 4.304955  | 2.054416  |
| 1  | 0.101893   | 4.714285  | 0.580194  |
| 1  | -0.905036  | 4.359506  | 1.831196  |
| 7  | 10.875891  | -4.689214 | -0.609584 |
| 1  | 11.589018  | -5.063201 | 0.009100  |
| 1  | 11.323223  | -3.986766 | -1.190580 |
| 1  | 10.588567  | -5.444719 | -1.224193 |
| 7  | 4.009792   | -1.115299 | 0.899472  |
| 1  | 3.561033   | -1.977817 | 1.195483  |
| 1  | 4.400335   | -0.696019 | 1.738932  |
| 1  | 4.806071   | -1.384749 | 0.304889  |
| 7  | -11.021842 | -4.483082 | -0.623696 |
| 1  | -10.742618 | -5.238735 | -1.241848 |
| 1  | -11.737316 | -4.852906 | -0.005216 |
| 1  | -11.463706 | -3.774225 | -1.201078 |
| 7  | -2.356217  | 0.716534  | -0.866703 |
| 1  | -2.916765  | 1.523098  | -1.129883 |
| 1  | -2.191849  | 0.193452  | -1.723111 |
| 1  | -2.948227  | 0.122692  | -0.261311 |
| 7  | -8.545996  | -3.281576 | 0.973046  |
| 1  | -9.340037  | -3.670993 | 0.457845  |
| 1  | -8.109308  | -4.048251 | 1.476426  |
| 1  | -8.923845  | -2.652602 | 1.675558  |
| 7  | -4.093543  | -1.032977 | 0.893063  |
| 1  | -4.889286  | -1.296404 | 0.295040  |
| 1  | -4.483341  | -0.583552 | 1.717117  |
| 1  | -3.670897  | -1.899211 | 1.215493  |
| 7  | 6.407782   | -1.936100 | -0.867610 |
| 1  | 6.906760   | -1.156176 | -1.285884 |
| 1  | 6.162893   | -2.561673 | -1.629830 |
| 1  | 7.077079   | -2.436666 | -0.270677 |
| 7  | -6.490538  | -1.834758 | -0.883653 |
| 1  | -6.970079  | -1.052256 | -1.319493 |
| 1  | -7.175282  | -2.312111 | -0.285232 |
| 1  | -6.250932  | -2.477519 | -1.633155 |
| 7  | 8.415150   | -3.454075 | 0.984780  |
| 1  | 8.801425   | -2.843411 | 1.698774  |
| 1  | 9.204316   | -3.854839 | 0.470798  |
| 1  | 7.956647   | -4.217093 | 1.474132  |
| 7  | 0.359436   | 5.989246  | -0.982545 |
| 1  | 1.267438   | 5.902843  | -1.430501 |
| 1  | 0.283771   | 6.955053  | -0.647585 |
| 1  | -0.333490  | 5.875465  | -1.717038 |
| 7  | 0.150213   | 8.984044  | 0.012559  |
| 1  | 0.331414   | 9.623565  | -0.755604 |
| 1  | 0.824566   | 9.199693  | 0.740835  |
| 1  | -0.766662  | 9.218790  | 0.381125  |

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Cartesian coordinates of the protonated ammonia pentadecamer

Cartesian coordinates of : Ca15\_1

-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.592130 | -0.388547 | -0.633880 |
| 1  | -1.026171 | -1.251909 | -1.033360 |
| 1  | 0.434573  | -0.343577 | -0.908274 |
| 1  | -1.079026 | 0.471530  | -0.961255 |
| 1  | -0.698059 | -0.410057 | 0.387244  |
| 7  | -2.046221 | 2.113004  | -1.184382 |
| 1  | -1.838492 | 2.930896  | -1.750942 |
| 1  | -2.715842 | 1.536825  | -1.709681 |
| 1  | -2.491354 | 2.439203  | -0.327021 |
| 7  | -1.697750 | -2.973366 | -1.386402 |
| 1  | -1.611365 | -3.264953 | -0.409429 |
| 1  | -2.694139 | -2.882410 | -1.569812 |
| 1  | -1.348534 | -3.721387 | -1.978699 |
| 7  | 1.595773  | -0.389060 | 1.837215  |
| 1  | 1.746993  | -0.630125 | 2.814358  |
| 1  | 2.465439  | 0.035923  | 1.507555  |
| 1  | 1.511628  | -1.275056 | 1.333921  |
| 7  | 2.094233  | -0.259469 | -1.532513 |
| 1  | 2.227003  | -0.784353 | -2.394648 |
| 1  | 2.346082  | 0.712988  | -1.746846 |
| 1  | 2.786929  | -0.613205 | -0.871744 |
| 7  | 3.902258  | 1.490596  | 0.465241  |
| 1  | 4.505490  | 1.988706  | 1.114787  |
| 1  | 4.321797  | 1.585870  | -0.457655 |
| 1  | 3.021272  | 2.005624  | 0.412902  |
| 7  | 2.531725  | 2.765117  | -2.136176 |
| 1  | 1.948868  | 2.997179  | -1.330179 |
| 1  | 1.992234  | 2.951487  | -2.976748 |
| 1  | 3.317882  | 3.408483  | -2.151631 |
| 7  | -3.491457 | -0.231602 | -2.458348 |
| 1  | -4.405042 | -0.147141 | -2.893816 |
| 1  | -3.602907 | -0.739816 | -1.575989 |
| 1  | -2.917205 | -0.791427 | -3.081883 |
| 7  | -3.605989 | -1.304340 | 0.473686  |
| 1  | -3.197062 | -2.159295 | 0.848149  |
| 1  | -4.579513 | -1.277130 | 0.764126  |
| 1  | -3.120880 | -0.547660 | 0.956553  |
| 7  | 4.347903  | -1.694711 | 0.381707  |
| 1  | 4.417325  | -0.695533 | 0.586109  |
| 1  | 5.125061  | -1.933274 | -0.228842 |
| 1  | 4.507331  | -2.189374 | 1.255792  |
| 7  | -1.085903 | -2.779330 | 1.707465  |
| 1  | -0.127012 | -2.853607 | 1.359942  |
| 1  | -1.198203 | -3.455934 | 2.457148  |
| 1  | -1.193097 | -1.852302 | 2.117051  |
| 7  | 1.490650  | -3.016599 | -0.099018 |
| 1  | 2.459836  | -2.685463 | -0.117309 |
| 1  | 1.068363  | -2.771945 | -0.991899 |
| 1  | 1.525227  | -4.032515 | -0.060176 |
| 7  | -2.768818 | 3.567556  | 1.700273  |
| 1  | -2.443826 | 3.724694  | 2.651418  |
| 1  | -3.780303 | 3.476109  | 1.759308  |
| 1  | -2.591788 | 4.434062  | 1.197587  |
| 7  | -1.476037 | 0.565291  | 2.186080  |
| 1  | -0.474953 | 0.568941  | 2.386602  |
| 1  | -1.963006 | 0.436741  | 3.069962  |
| 1  | -1.728556 | 1.495687  | 1.845257  |
| 7  | 0.761588  | 2.414820  | 0.481838  |
| 1  | 0.581633  | 3.094082  | 1.216992  |
| 1  | 0.889697  | 1.509440  | 0.938288  |
| 1  | -0.093114 | 2.349453  | -0.072697 |

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Cartesian coordinates of : BCa15\_1-----  
Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.026377  | 0.458035  | -0.920372 |
| 1  | -0.193177 | 1.395387  | -1.313155 |
| 1  | 0.534394  | 0.550994  | 0.002881  |
| 1  | -0.889492 | -0.009758 | -0.807013 |
| 1  | 0.628718  | -0.102897 | -1.569887 |
| 7  | -2.884689 | -0.024196 | -1.038724 |
| 1  | -3.033780 | 0.700701  | -0.337612 |
| 1  | -3.309974 | 0.302572  | -1.901994 |
| 1  | -3.386349 | -0.855598 | -0.728152 |
| 7  | -1.087189 | 3.006307  | -1.953649 |
| 1  | -1.014934 | 2.963780  | -2.967476 |
| 1  | -2.089768 | 3.036833  | -1.730341 |
| 1  | -0.697773 | 3.907071  | -1.686373 |
| 7  | 1.762413  | -1.253792 | -2.462915 |
| 1  | 1.311691  | -2.165978 | -2.455761 |
| 1  | 2.594611  | -1.315757 | -1.870097 |
| 1  | 2.068460  | -1.072734 | -3.414325 |
| 7  | -3.860129 | -2.742174 | 0.452984  |
| 1  | -4.634726 | -3.116811 | -0.089076 |
| 1  | -4.234024 | -1.991234 | 1.044452  |
| 1  | -3.560845 | -3.491884 | 1.071870  |
| 7  | -4.532285 | -0.089838 | 1.969798  |
| 1  | -5.421035 | 0.298623  | 1.664855  |
| 1  | -4.605150 | -0.203792 | 2.977440  |
| 1  | -3.820770 | 0.622455  | 1.800835  |
| 7  | 1.539465  | 0.522710  | 1.478254  |
| 1  | 2.507334  | 0.844979  | 1.426000  |
| 1  | 1.116794  | 0.908805  | 2.317175  |
| 1  | 1.548530  | -0.494184 | 1.572582  |
| 7  | 1.232152  | -2.444578 | 0.499553  |
| 1  | 1.363448  | -3.360209 | 0.920522  |
| 1  | 0.527862  | -2.549391 | -0.238221 |
| 1  | 2.115879  | -2.184071 | 0.062307  |
| 7  | 4.158322  | -1.190336 | -0.326811 |
| 1  | 4.491641  | -1.910255 | 0.310286  |
| 1  | 4.115208  | -0.323437 | 0.214692  |
| 1  | 4.905091  | -1.057775 | -1.004981 |
| 7  | -1.203601 | -2.680111 | -1.513234 |
| 1  | -1.182354 | -3.547830 | -2.043306 |
| 1  | -1.423900 | -1.935653 | -2.170554 |
| 1  | -2.010333 | -2.739284 | -0.886616 |
| 7  | -1.335270 | -1.016648 | 1.708919  |
| 1  | -2.034112 | -1.427973 | 1.090678  |
| 1  | -1.593089 | -1.294724 | 2.652683  |
| 1  | -0.446858 | -1.473849 | 1.492238  |
| 7  | 4.608630  | 1.561546  | 1.321003  |
| 1  | 4.705099  | 1.632648  | 2.331095  |
| 1  | 4.385880  | 2.496668  | 0.989158  |
| 1  | 5.541171  | 1.336382  | 0.957310  |
| 7  | -4.011478 | 3.122481  | -0.854253 |
| 1  | -4.809440 | 2.579132  | -1.170987 |
| 1  | -4.326813 | 4.086287  | -0.788875 |
| 1  | -3.770615 | 2.808583  | 0.086230  |
| 7  | 7.494585  | 0.825319  | 0.271820  |
| 1  | 7.777652  | -0.127554 | 0.481811  |
| 1  | 8.127215  | 1.435116  | 0.782660  |
| 1  | 7.680818  | 0.977749  | -0.715235 |
| 7  | -1.999712 | 1.939250  | 1.292316  |
| 1  | -1.580913 | 1.020097  | 1.491560  |
| 1  | -1.884679 | 2.517036  | 2.121125  |
| 1  | -1.445726 | 2.372923  | 0.554767  |

Cartesian coordinates of : BDC15

Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z        |
|----|-----------|-----------|----------|
| 7  | -0.404926 | -0.631767 | 0.460898 |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | 0.040855   | -0.717303 | 1.400313  |
| 1 | 0.258383   | -1.087738 | -0.204732 |
| 1 | -1.336370  | -1.100372 | 0.438735  |
| 1 | -0.597694  | 0.370654  | 0.202010  |
| 7 | -3.195818  | -1.418921 | 0.209430  |
| 1 | -3.703775  | -1.755965 | 1.022648  |
| 1 | -3.594371  | -0.504861 | -0.024122 |
| 1 | -3.431116  | -2.045791 | -0.555187 |
| 7 | 1.222015   | -1.149746 | 2.821632  |
| 1 | 1.470606   | -0.363897 | 3.415982  |
| 1 | 0.896549   | -1.887028 | 3.440720  |
| 1 | 2.087669   | -1.481500 | 2.379813  |
| 7 | -1.416690  | 1.924493  | -0.301563 |
| 1 | -1.146080  | 2.257318  | -1.222893 |
| 1 | -1.311389  | 2.713205  | 0.343440  |
| 1 | -2.411557  | 1.691329  | -0.349198 |
| 7 | -4.636496  | 1.368075  | -0.463697 |
| 1 | -4.748868  | 1.728329  | -1.408111 |
| 1 | -4.794362  | 2.155518  | 0.160355  |
| 1 | -5.412793  | 0.709534  | -0.306355 |
| 7 | 9.007551   | 0.754122  | -1.660223 |
| 1 | 8.843104   | 1.728456  | -1.896401 |
| 1 | 9.961524   | 0.690074  | -1.293881 |
| 1 | 8.989366   | 0.238856  | -2.535609 |
| 7 | 1.690931   | -2.087192 | -0.916206 |
| 1 | 1.532574   | -2.638471 | -1.754777 |
| 1 | 2.525439   | -1.513336 | -1.075530 |
| 1 | 1.931033   | -2.735939 | -0.170095 |
| 7 | 6.889188   | -0.315626 | 0.347560  |
| 1 | 7.604177   | 0.039632  | -0.300748 |
| 1 | 6.925990   | 0.273066  | 1.175198  |
| 1 | 7.190858   | -1.241904 | 0.637687  |
| 7 | 3.918181   | -2.022229 | 1.442468  |
| 1 | 4.076732   | -1.540789 | 0.555677  |
| 1 | 4.161386   | -2.998786 | 1.297253  |
| 1 | 4.611002   | -1.655001 | 2.089774  |
| 7 | -6.855129  | -0.715874 | 0.023312  |
| 1 | -7.030149  | -0.943383 | 0.998212  |
| 1 | -6.734784  | -1.601088 | -0.461015 |
| 1 | -7.716733  | -0.290440 | -0.342531 |
| 7 | 4.319360   | -0.351259 | -1.359374 |
| 1 | 4.585538   | -0.652455 | -2.293461 |
| 1 | 5.190861   | -0.275740 | -0.816973 |
| 1 | 3.951328   | 0.591330  | -1.457944 |
| 7 | -9.424623  | 0.627756  | -1.102464 |
| 1 | -9.572484  | 1.542335  | -0.685577 |
| 1 | -10.271616 | 0.078523  | -0.931748 |
| 1 | -9.361822  | 0.775341  | -2.105666 |
| 7 | 11.981348  | 0.563338  | -0.556201 |
| 1 | 12.630478  | 1.066064  | -1.153937 |
| 1 | 12.307045  | -0.397221 | -0.506014 |
| 1 | 12.070259  | 0.956047  | 0.376029  |
| 7 | -12.073467 | -1.053682 | -0.592388 |
| 1 | -12.890140 | -0.579993 | -0.966575 |
| 1 | -12.245550 | -1.206640 | 0.396634  |
| 1 | -12.032776 | -1.968314 | -1.031693 |
| 7 | -1.077674  | 4.422198  | 1.638412  |
| 1 | -1.520909  | 5.244909  | 1.240402  |
| 1 | -0.099127  | 4.654304  | 1.780169  |
| 1 | -1.484560  | 4.283330  | 2.558540  |

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Cartesian coordinates of : BC15\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y        | Z         |
|----|-----------|----------|-----------|
| 7  | 0.107667  | 0.162196 | -0.237448 |
| 1  | 0.351379  | 0.518462 | 0.711456  |
| 1  | -0.857150 | 0.480084 | -0.513021 |
| 1  | 0.822259  | 0.579260 | -0.870686 |

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|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.149077  | -0.886623 | -0.262589 |
| 7 | 2.263965  | 1.667144  | -1.501674 |
| 1 | 2.193657  | 2.080919  | -2.426763 |
| 1 | 2.285114  | 2.430451  | -0.829106 |
| 1 | 3.176081  | 1.206182  | -1.435716 |
| 7 | 1.191546  | 1.420894  | 2.169904  |
| 1 | 0.674387  | 2.230624  | 2.500773  |
| 1 | 1.368852  | 0.839246  | 2.983984  |
| 1 | 2.100192  | 1.754630  | 1.829155  |
| 7 | 0.106746  | -2.732223 | -0.325628 |
| 1 | 0.490472  | -3.112787 | -1.186699 |
| 1 | -0.870837 | -3.053856 | -0.266697 |
| 1 | 0.609823  | -3.182762 | 0.434201  |
| 7 | -2.556006 | 0.961833  | -0.992932 |
| 1 | -3.193317 | 0.178891  | -0.871547 |
| 1 | -2.923133 | 1.740083  | -0.425369 |
| 1 | -2.635753 | 1.245450  | -1.965950 |
| 7 | -2.776792 | -3.777564 | -0.122965 |
| 1 | -2.671393 | -4.774037 | 0.105758  |
| 1 | -3.347575 | -3.363994 | 0.608850  |
| 1 | -3.323184 | -3.726992 | -0.978166 |
| 7 | -3.719961 | 3.300312  | 0.622438  |
| 1 | -3.090218 | 4.083397  | 0.772243  |
| 1 | -4.081969 | 3.044222  | 1.536651  |
| 1 | -4.513176 | 3.653995  | 0.073225  |
| 7 | 4.041767  | 2.308780  | 1.120696  |
| 1 | 4.402872  | 1.697417  | 0.385984  |
| 1 | 4.612731  | 2.138839  | 1.944565  |
| 1 | 4.238338  | 3.264261  | 0.834098  |
| 7 | -2.398535 | -6.793461 | 0.562504  |
| 1 | -1.672550 | -7.213023 | -0.011067 |
| 1 | -3.253186 | -7.336402 | 0.410804  |
| 1 | -2.121715 | -6.937645 | 1.529293  |
| 7 | -6.113470 | 4.349722  | -1.079945 |
| 1 | -6.687312 | 5.023831  | -0.565770 |
| 1 | -6.727280 | 3.593914  | -1.369758 |
| 1 | -5.801892 | 4.810273  | -1.930160 |
| 7 | 5.145990  | 0.296801  | -1.219814 |
| 1 | 5.494149  | 0.482278  | -2.157021 |
| 1 | 4.912098  | -0.692173 | -1.192258 |
| 1 | 5.938562  | 0.434864  | -0.578865 |
| 7 | 7.415509  | 0.912808  | 0.793333  |
| 1 | 8.307037  | 0.611297  | 0.387110  |
| 1 | 7.343130  | 0.468433  | 1.704382  |
| 1 | 7.491969  | 1.911951  | 0.962934  |
| 7 | 10.178265 | -0.005365 | -0.441999 |
| 1 | 10.929139 | 0.078526  | 0.236895  |
| 1 | 10.445877 | 0.551458  | -1.248165 |
| 1 | 10.160559 | -0.974512 | -0.745222 |
| 7 | -7.900259 | 6.456837  | 0.493830  |
| 1 | -8.479670 | 6.018095  | 1.203052  |
| 1 | -8.524033 | 6.960106  | -0.129830 |
| 1 | -7.327456 | 7.150161  | 0.965371  |
| 7 | -5.036288 | -8.509052 | 0.110902  |
| 1 | -5.328218 | -8.519986 | -0.861649 |
| 1 | -5.816904 | -8.148821 | 0.651338  |
| 1 | -4.900853 | -9.475620 | 0.391537  |

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Cartesian coordinates of : BC15\_2

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.244269 | 1.046739  | 0.358739  |
| 1  | -0.338502 | 0.394398  | 1.165608  |
| 1  | 0.623417  | 0.817605  | -0.194678 |
| 1  | -1.096827 | 0.881583  | -0.214143 |
| 1  | -0.208496 | 2.041587  | 0.692983  |
| 7  | -2.766298 | 0.125538  | -0.818180 |
| 1  | -2.694943 | -0.431636 | -1.665230 |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | -3.065865  | -0.507914 | -0.073332 |
| 1 | -3.534439  | 0.774279  | -0.966412 |
| 7 | -0.986094  | -0.954578 | 2.358730  |
| 1 | -1.914800  | -1.221823 | 2.018548  |
| 1 | -0.410343  | -1.791786 | 2.361233  |
| 1 | -1.088401  | -0.667596 | 3.327928  |
| 7 | -0.116510  | 3.789395  | 1.288073  |
| 1 | -0.027651  | 4.448368  | 0.501468  |
| 1 | 0.683962   | 3.945081  | 1.895292  |
| 1 | -0.935623  | 4.072675  | 1.819418  |
| 7 | -3.926845  | -1.879960 | 1.482905  |
| 1 | -4.303076  | -1.706641 | 2.412119  |
| 1 | -3.771904  | -2.883754 | 1.426306  |
| 1 | -4.686447  | -1.665464 | 0.820834  |
| 7 | 0.147869   | 5.781993  | -1.051015 |
| 1 | -0.642477  | 5.747899  | -1.688609 |
| 1 | 0.203306   | 6.740164  | -0.692661 |
| 1 | 0.978450   | 5.627678  | -1.615508 |
| 7 | 2.139615   | 0.400820  | -1.108931 |
| 1 | 1.969345   | -0.087135 | -1.984473 |
| 1 | 2.697270   | 1.217863  | -1.344089 |
| 1 | 2.740080   | -0.213217 | -0.536543 |
| 7 | 8.625101   | -3.317499 | 0.486058  |
| 1 | 9.549646   | -3.363393 | 0.049650  |
| 1 | 8.767393   | -3.125608 | 1.473347  |
| 1 | 8.218361   | -4.246405 | 0.427319  |
| 7 | 3.985039   | -1.388227 | 0.542167  |
| 1 | 4.906725   | -1.305308 | 0.092534  |
| 1 | 3.749049   | -2.376648 | 0.546332  |
| 1 | 4.105621   | -1.119220 | 1.514605  |
| 7 | -6.146935  | -1.208375 | -0.545315 |
| 1 | -5.923211  | -1.335325 | -1.528463 |
| 1 | -6.575787  | -0.290576 | -0.463800 |
| 1 | -6.874147  | -1.897694 | -0.313055 |
| 7 | 6.761880   | -1.168638 | -0.818982 |
| 1 | 6.732063   | -1.352182 | -1.817762 |
| 1 | 7.383087   | -1.871247 | -0.401064 |
| 1 | 7.213800   | -0.265809 | -0.705950 |
| 7 | -8.288280  | -3.318571 | 0.234558  |
| 1 | -7.934054  | -4.266177 | 0.140943  |
| 1 | -9.139231  | -3.258800 | -0.331805 |
| 1 | -8.568191  | -3.210662 | 1.205250  |
| 7 | 0.331165   | 8.755979  | 0.029952  |
| 1 | -0.490491  | 9.028540  | 0.561036  |
| 1 | 0.421000   | 9.416868  | -0.736077 |
| 1 | 1.134178   | 8.894597  | 0.636094  |
| 7 | -10.948026 | -3.170740 | -1.497011 |
| 1 | -11.579947 | -3.929062 | -1.258153 |
| 1 | -10.763947 | -3.239761 | -2.493284 |
| 1 | -11.455146 | -2.303608 | -1.348180 |
| 7 | 11.496293  | -3.454012 | -0.880818 |
| 1 | 12.153105  | -4.030149 | -0.363356 |
| 1 | 11.907003  | -2.528627 | -0.958298 |
| 1 | 11.441156  | -3.835002 | -1.820436 |

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Cartesian coordinates of : BL15

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.003578 | 0.555490  | 0.717734  |
| 1  | 0.036990  | 1.553536  | 1.080799  |
| 1  | -0.897115 | 0.401073  | 0.157931  |
| 1  | 0.854490  | 0.343948  | 0.122075  |
| 1  | -0.008144 | -0.081846 | 1.511749  |
| 7  | 2.302659  | -0.054110 | -0.787550 |
| 1  | 2.856496  | 0.763003  | -1.031648 |
| 1  | 2.907217  | -0.669270 | -0.217446 |
| 1  | 2.120068  | -0.544660 | -1.659299 |
| 7  | 0.108664  | 3.218912  | 1.685852  |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | 0.949562   | 3.413634  | 2.223708  |
| 1 | 0.099256   | 3.885978  | 0.897041  |
| 1 | -0.674256  | 3.465453  | 2.286293  |
| 7 | 11.001825  | -5.241940 | -0.794945 |
| 1 | 11.716007  | -5.652058 | -0.200893 |
| 1 | 11.453269  | -4.522626 | -1.351596 |
| 1 | 10.695585  | -5.966665 | -1.436876 |
| 7 | 4.077103   | -1.867708 | 0.873574  |
| 1 | 3.668837   | -2.759687 | 1.139326  |
| 1 | 4.449878   | -1.460487 | 1.726901  |
| 1 | 4.883312   | -2.079113 | 0.269201  |
| 7 | -10.950187 | -5.324257 | -0.814157 |
| 1 | -10.630480 | -6.042429 | -1.456880 |
| 1 | -11.663063 | -5.745784 | -0.226562 |
| 1 | -11.406972 | -4.608450 | -1.370975 |
| 7 | -2.402424  | 0.092136  | -0.692337 |
| 1 | -2.968106  | 0.927763  | -0.817704 |
| 1 | -2.277887  | -0.308632 | -1.618505 |
| 1 | -2.970880  | -0.578750 | -0.148574 |
| 7 | -8.546709  | -4.092882 | 0.868618  |
| 1 | -9.318651  | -4.492862 | 0.328601  |
| 1 | -8.096547  | -4.858171 | 1.362113  |
| 1 | -8.956404  | -3.492406 | 1.578167  |
| 7 | -4.068876  | -1.886446 | 0.890131  |
| 1 | -4.872794  | -2.102071 | 0.284213  |
| 1 | -4.448028  | -1.538419 | 1.766540  |
| 1 | -3.619577  | -2.771985 | 1.106587  |
| 7 | 6.508151   | -2.517996 | -0.922090 |
| 1 | 6.976793   | -1.701563 | -1.304150 |
| 1 | 6.286231   | -3.117375 | -1.711855 |
| 1 | 7.195931   | -3.019077 | -0.347162 |
| 7 | -6.494105  | -2.545649 | -0.910218 |
| 1 | -6.968236  | -1.729650 | -1.286385 |
| 1 | -7.178270  | -3.055158 | -0.338377 |
| 1 | -6.268901  | -3.138233 | -1.704171 |
| 7 | 8.571497   | -4.037240 | 0.868494  |
| 1 | 8.968745   | -3.429097 | 1.578597  |
| 1 | 9.352005   | -4.428148 | 0.334180  |
| 1 | 8.129072   | -4.807209 | 1.361703  |
| 7 | 0.080528   | 5.253747  | -0.578662 |
| 1 | 0.921083   | 5.271997  | -1.149415 |
| 1 | 0.010098   | 6.171133  | -0.119690 |
| 1 | -0.701017  | 5.184014  | -1.224272 |
| 7 | -0.123405  | 8.003720  | 0.859342  |
| 1 | -0.102511  | 8.784918  | 0.197657  |
| 1 | 0.643873   | 8.144149  | 1.510329  |
| 1 | -0.979053  | 8.093956  | 1.399636  |
| 7 | -0.061665  | 10.452563 | -1.163533 |
| 1 | -0.843918  | 10.433658 | -1.810815 |
| 1 | 0.785933   | 10.466684 | -1.722655 |
| 1 | -0.106272  | 11.338606 | -0.669210 |

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Cartesian coordinates of : P\_NH3\_N15\_1.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.173285 | -1.395017 | -1.477266 |
| 1  | -0.937908 | -0.098149 | -2.603781 |
| 1  | -2.376838 | -2.141705 | -2.138167 |
| 1  | -1.859627 | -1.856923 | -0.620387 |
| 1  | -3.062218 | -0.940612 | -1.264465 |
| 7  | 0.707270  | -2.930546 | -1.459749 |
| 1  | 0.667909  | -3.750185 | -2.060021 |
| 1  | 0.370928  | -2.143848 | -2.011957 |
| 1  | 0.014485  | -3.063033 | -0.717516 |
| 7  | 1.617745  | 0.515508  | -0.713830 |
| 1  | 2.352791  | -0.213463 | -0.895798 |
| 1  | 2.085087  | 1.402310  | -0.479978 |
| 1  | 1.019201  | 0.242737  | 0.111524  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -0.266798 | 0.587756  | -2.968735 |
| 1 | 1.017217  | 0.624570  | -1.559619 |
| 1 | -0.045597 | 0.339122  | -3.928789 |
| 1 | -0.755415 | 1.479652  | -2.991161 |
| 7 | -1.148073 | -3.054807 | 1.134074  |
| 1 | -0.258564 | -2.986684 | 1.630573  |
| 1 | -1.524607 | -3.982334 | 1.308207  |
| 1 | -1.791248 | -2.381705 | 1.553205  |
| 7 | 2.034747  | -2.531107 | 1.510805  |
| 1 | 2.680982  | -1.736647 | 1.509610  |
| 1 | 1.871404  | -2.797010 | 0.539824  |
| 1 | 2.497355  | -3.307807 | 1.973856  |
| 7 | 3.525815  | -1.562931 | -1.293076 |
| 1 | 2.841322  | -2.311609 | -1.418465 |
| 1 | 4.092000  | -1.789172 | -0.480147 |
| 1 | 4.139715  | -1.548886 | -2.101914 |
| 7 | 0.104513  | -0.165884 | 1.618462  |
| 1 | -0.884028 | -0.418367 | 1.574326  |
| 1 | 0.188812  | 0.545667  | 2.339361  |
| 1 | 0.627333  | -0.990892 | 1.923510  |
| 7 | -3.100577 | -0.460842 | 1.681608  |
| 1 | -3.752303 | -0.895563 | 2.329911  |
| 1 | -3.605849 | -0.301906 | 0.809340  |
| 1 | -2.868028 | 0.458581  | 2.059911  |
| 7 | -5.044293 | 0.158528  | -0.954448 |
| 1 | -5.671706 | -0.639333 | -0.884917 |
| 1 | -5.070994 | 0.456429  | -1.926745 |
| 1 | -5.475595 | 0.905890  | -0.416045 |
| 7 | -1.964350 | 2.424387  | 2.859884  |
| 1 | -2.800601 | 3.003111  | 2.878389  |
| 1 | -1.185422 | 3.059556  | 2.702841  |
| 1 | -1.851040 | 2.058573  | 3.802269  |
| 7 | 3.174725  | 3.019858  | 0.187371  |
| 1 | 2.403984  | 3.449745  | -0.337906 |
| 1 | 4.035401  | 3.226303  | -0.312921 |
| 1 | 3.240150  | 3.500643  | 1.080518  |
| 7 | 0.665679  | 3.521822  | -1.513638 |
| 1 | -0.115299 | 2.947655  | -1.178027 |
| 1 | 0.874377  | 3.235994  | -2.466590 |
| 1 | 0.338909  | 4.482694  | -1.564557 |
| 7 | -1.624506 | 1.646995  | -0.376010 |
| 1 | -1.407677 | 0.659007  | -0.504067 |
| 1 | -2.576316 | 1.764850  | -0.717664 |
| 1 | -1.658509 | 1.803248  | 0.631589  |
| 7 | 3.796958  | 0.134427  | 1.679417  |
| 1 | 3.644941  | 0.329418  | 2.665844  |
| 1 | 3.597747  | 0.999592  | 1.174042  |
| 1 | 4.794348  | -0.036547 | 1.578865  |

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Cartesian coordinates of : P\_NH3\_N15\_13.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.129767  | 1.055479  | 0.544132  |
| 1  | 0.753186  | 1.391685  | -0.226490 |
| 1  | 0.681081  | 0.275233  | 0.955822  |
| 1  | -0.049771 | 1.807132  | 1.246051  |
| 1  | -0.781567 | 0.671076  | 0.163193  |
| 7  | -0.602557 | 1.641705  | -2.764213 |
| 1  | -1.228266 | 1.714552  | -3.561854 |
| 1  | 0.238516  | 2.173349  | -2.990417 |
| 1  | -1.060695 | 2.116190  | -1.990376 |
| 7  | 0.416911  | -1.280702 | -2.039071 |
| 1  | 0.227651  | -1.810168 | -2.887428 |
| 1  | -0.167568 | -1.682994 | -1.302828 |
| 1  | 0.063621  | -0.334525 | -2.221400 |
| 7  | 2.226916  | 1.369446  | -1.404168 |
| 1  | 2.077847  | 0.461841  | -1.845239 |
| 1  | 2.298401  | 2.060954  | -2.148885 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.112472  | 1.322658  | -0.898845 |
| 7 | -0.423979 | 3.163559  | 2.510650  |
| 1 | 0.080945  | 4.026992  | 2.329975  |
| 1 | -0.180638 | 2.867910  | 3.462582  |
| 1 | -1.411325 | 3.405277  | 2.519103  |
| 7 | -0.531708 | -2.766436 | 0.608624  |
| 1 | 0.126694  | -3.436698 | 0.208846  |
| 1 | 0.009147  | -2.206499 | 1.265770  |
| 1 | -1.213644 | -3.295236 | 1.145252  |
| 7 | 2.112379  | -1.014673 | 0.779154  |
| 1 | 1.883663  | -1.287133 | -0.178809 |
| 1 | 2.353042  | -1.866148 | 1.295009  |
| 1 | 2.940489  | -0.422703 | 0.722178  |
| 7 | -2.234316 | -0.172647 | -0.443902 |
| 1 | -3.166780 | 0.073647  | -0.089468 |
| 1 | -2.035952 | -1.141072 | -0.188215 |
| 1 | -2.269707 | -0.139315 | -1.460011 |
| 7 | 4.945433  | 0.826772  | 0.387972  |
| 1 | 5.007908  | 0.865471  | 1.401813  |
| 1 | 5.475048  | 1.621244  | 0.039011  |
| 1 | 5.448590  | -0.006288 | 0.094527  |
| 7 | 1.934538  | 3.354470  | -4.034690 |
| 1 | 2.045267  | 2.794055  | -4.875686 |
| 1 | 2.827729  | 3.813664  | -3.876142 |
| 1 | 1.273158  | 4.092883  | -4.260557 |
| 7 | 0.305063  | 2.278618  | 5.436724  |
| 1 | 0.873667  | 2.978040  | 5.905228  |
| 1 | 0.823962  | 1.406070  | 5.468707  |
| 1 | -0.526302 | 2.148503  | 6.005807  |
| 7 | 2.346805  | -3.899962 | 1.934713  |
| 1 | 1.623464  | -4.225327 | 2.568944  |
| 1 | 3.213362  | -4.341678 | 2.226639  |
| 1 | 2.118763  | -4.240949 | 1.000220  |
| 7 | -5.069197 | 0.600418  | 0.607759  |
| 1 | -5.303712 | 1.577661  | 0.458344  |
| 1 | -5.169065 | 0.431287  | 1.604669  |
| 1 | -5.791049 | 0.045996  | 0.138090  |
| 7 | 1.804410  | -4.049032 | -1.239974 |
| 1 | 1.225173  | -4.629944 | -1.840749 |
| 1 | 2.761473  | -4.361948 | -1.380497 |
| 1 | 1.746260  | -3.095245 | -1.598550 |
| 7 | -7.363741 | -1.078161 | -0.809824 |
| 1 | -7.646769 | -1.876829 | -0.249876 |
| 1 | -7.092245 | -1.436501 | -1.720370 |
| 1 | -8.192594 | -0.508143 | -0.950287 |

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Cartesian coordinates of : P\_NH3\_N15\_2.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -2.819139 | 0.886729  | 0.117725  |
| 1  | -2.251322 | 0.485870  | 0.896494  |
| 1  | -3.143905 | 1.849955  | 0.355782  |
| 1  | -2.248373 | 0.901828  | -0.767064 |
| 1  | -3.634471 | 0.239564  | 0.010494  |
| 7  | -1.252391 | 0.958016  | -2.311829 |
| 1  | -0.236564 | 0.931410  | -2.165732 |
| 1  | -1.470738 | 0.224636  | -2.982257 |
| 1  | -1.474071 | 1.842835  | -2.779145 |
| 7  | -1.488290 | -0.749591 | 2.097790  |
| 1  | -0.955360 | -0.523366 | 2.931242  |
| 1  | -2.238258 | -1.383026 | 2.364243  |
| 1  | -0.887908 | -1.266222 | 1.450938  |
| 7  | -4.826406 | -1.202985 | 0.129973  |
| 1  | -5.581447 | -1.099192 | 0.801868  |
| 1  | -4.218451 | -1.965872 | 0.457377  |
| 1  | -5.253359 | -1.509676 | -0.739584 |
| 7  | -3.727879 | 3.601609  | 0.781106  |
| 1  | -4.340396 | 3.982554  | 0.064945  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -4.243454 | 3.643806  | 1.667283  |
| 1 | -2.946027 | 4.245996  | 0.862917  |
| 7 | -2.740580 | -3.377653 | 0.804365  |
| 1 | -3.069590 | -4.115452 | 0.175170  |
| 1 | -1.868115 | -3.006185 | 0.426126  |
| 1 | -2.511559 | -3.835457 | 1.682708  |
| 7 | -5.317179 | 3.808204  | 3.484342  |
| 1 | -5.429799 | 4.782437  | 3.749446  |
| 1 | -4.850152 | 3.344686  | 4.258135  |
| 1 | -6.250127 | 3.411161  | 3.422867  |
| 7 | -0.095531 | -1.851091 | -0.493416 |
| 1 | -0.365460 | -0.997545 | -0.980016 |
| 1 | -0.114502 | -2.595326 | -1.186327 |
| 1 | 0.886099  | -1.726757 | -0.227997 |
| 7 | 2.922064  | -1.460167 | 0.488880  |
| 1 | 3.671770  | -0.771185 | 0.336081  |
| 1 | 3.313949  | -2.369594 | 0.257207  |
| 1 | 2.739852  | -1.477978 | 1.489061  |
| 7 | 5.119090  | 0.615368  | -0.120262 |
| 1 | 5.271436  | 0.762146  | -1.114200 |
| 1 | 5.982807  | 0.205885  | 0.258112  |
| 1 | 5.021328  | 1.536901  | 0.296614  |
| 7 | 1.832568  | 0.605740  | -1.810061 |
| 1 | 2.298820  | 1.486405  | -1.609570 |
| 1 | 2.241490  | 0.256050  | -2.672708 |
| 1 | 2.115539  | -0.042146 | -1.072924 |
| 7 | 7.682551  | -0.705324 | 1.050780  |
| 1 | 7.568040  | -0.896869 | 2.041909  |
| 1 | 8.526934  | -0.135327 | 0.949857  |
| 1 | 7.871034  | -1.598541 | 0.604903  |
| 7 | 10.335021 | 1.022907  | 0.751540  |
| 1 | 11.119908 | 0.569365  | 1.209374  |
| 1 | 10.243822 | 1.946800  | 1.162920  |
| 1 | 10.594113 | 1.155165  | -0.221378 |
| 7 | -3.912734 | -5.759458 | -0.974202 |
| 1 | -4.056171 | -5.610403 | -1.968382 |
| 1 | -4.817097 | -5.997463 | -0.577638 |
| 1 | -3.324114 | -6.582021 | -0.881261 |
| 7 | -1.947742 | 3.606826  | -3.952286 |
| 1 | -2.916839 | 3.655260  | -4.252373 |
| 1 | -1.381054 | 3.559514  | -4.794117 |
| 1 | -1.732226 | 4.491471  | -3.502522 |

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Cartesian coordinates of : P\_NH3\_N15\_14.log

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Atomic number (AN) and Cartesian coordinates

| AN | X          | Y         | Z         |
|----|------------|-----------|-----------|
| 7  | -0.065282  | 0.220519  | -0.032660 |
| 1  | 0.003980   | 0.963902  | -0.725957 |
| 1  | -0.952236  | -0.405019 | -0.246810 |
| 1  | 0.868171   | -0.373349 | -0.046112 |
| 1  | -0.179147  | 0.655374  | 0.881688  |
| 7  | 2.256938   | -1.180812 | -0.095461 |
| 1  | 2.254214   | -1.951011 | -0.760405 |
| 1  | 3.014646   | -0.528168 | -0.385324 |
| 1  | 2.538575   | -1.577515 | 0.798381  |
| 7  | -14.225903 | 1.173411  | 0.501393  |
| 1  | -15.131367 | 0.732856  | 0.320417  |
| 1  | -14.177096 | 1.367236  | 1.497237  |
| 1  | -14.228347 | 2.073167  | 0.030154  |
| 7  | -11.761058 | -0.556930 | -0.372920 |
| 1  | -12.582249 | -0.006204 | -0.098453 |
| 1  | -11.883815 | -1.490357 | 0.008468  |
| 1  | -11.786288 | -0.651919 | -1.383944 |
| 7  | 4.443863   | 0.666815  | -0.843686 |
| 1  | 4.350012   | 1.657024  | -0.634386 |
| 1  | 4.746796   | 0.611098  | -1.812619 |
| 1  | 5.226310   | 0.314753  | -0.270322 |
| 7  | -6.785612  | -0.141977 | -0.988268 |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | -7.587690  | 0.219378  | -0.453507 |
| 1 | -6.680662  | 0.457184  | -1.802242 |
| 1 | -7.057232  | -1.055816 | -1.340364 |
| 7 | -2.275509  | -1.280989 | -0.502619 |
| 1 | -2.601586  | -1.271147 | -1.466588 |
| 1 | -2.167085  | -2.260265 | -0.248562 |
| 1 | -3.049225  | -0.896353 | 0.078094  |
| 7 | -9.199838  | 0.908314  | 0.628080  |
| 1 | -10.038028 | 0.412414  | 0.300095  |
| 1 | -9.130799  | 0.746577  | 1.628719  |
| 1 | -9.379506  | 1.901414  | 0.510278  |
| 7 | -4.518840  | -0.154368 | 1.064543  |
| 1 | -5.279932  | -0.146434 | 0.367900  |
| 1 | -4.456429  | 0.788403  | 1.439185  |
| 1 | -4.832118  | -0.742286 | 1.832593  |
| 7 | 6.782929   | -0.398733 | 0.809552  |
| 1 | 6.839387   | -1.405394 | 0.936301  |
| 1 | 6.899051   | 0.011055  | 1.732253  |
| 1 | 7.605808   | -0.122665 | 0.256045  |
| 7 | 9.258163   | 0.431844  | -0.846052 |
| 1 | 9.318118   | 0.002512  | -1.764938 |
| 1 | 10.093935  | 0.140595  | -0.323672 |
| 1 | 9.334698   | 1.434321  | -0.992792 |
| 7 | -17.030555 | -0.221085 | -0.081166 |
| 1 | -17.023186 | -1.184558 | 0.239111  |
| 1 | -17.227416 | -0.239107 | -1.077089 |
| 1 | -17.814714 | 0.239191  | 0.370678  |
| 7 | 11.799301  | -0.439076 | 0.730431  |
| 1 | 12.618165  | 0.064875  | 0.372138  |
| 1 | 11.997803  | -1.431935 | 0.648524  |
| 1 | 11.732911  | -0.238887 | 1.724082  |
| 7 | 14.262834  | 1.127709  | -0.415688 |
| 1 | 14.218526  | 1.138945  | -1.430344 |
| 1 | 15.167428  | 0.727854  | -0.153982 |
| 1 | 14.262932  | 2.097598  | -0.114129 |
| 7 | 17.059664  | -0.138916 | 0.434118  |
| 1 | 17.169304  | -1.075062 | 0.056581  |
| 1 | 17.113950  | -0.216425 | 1.445056  |
| 1 | 17.863774  | 0.402062  | 0.131365  |

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Cartesian coordinates of the protonated ammonia hexadecamer

Cartesian coordinates of : Ca16\_1

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 1.697894  | -2.110945 | 1.832362  |
| 1  | 1.069755  | -0.330240 | 2.630708  |
| 1  | 1.659228  | -2.820830 | 2.559390  |
| 1  | 1.141577  | -2.465552 | 1.053097  |
| 1  | 2.665355  | -2.054680 | 1.515027  |
| 7  | -1.680621 | -1.930275 | 1.908456  |
| 1  | -1.934320 | -2.560049 | 2.665698  |
| 1  | -1.060910 | -1.229288 | 2.311717  |
| 1  | -1.108085 | -2.470640 | 1.252108  |
| 7  | -1.304257 | 1.241813  | 0.786199  |
| 1  | -2.302469 | 0.964137  | 0.973680  |
| 1  | -1.237485 | 2.271198  | 0.618219  |
| 1  | -0.942678 | 0.690332  | -0.031122 |
| 7  | 0.645484  | 0.580452  | 2.854117  |
| 1  | -0.707382 | 1.008601  | 1.611227  |
| 1  | 0.481347  | 0.618838  | 3.856199  |
| 1  | 1.344592  | 1.287529  | 2.636799  |
| 7  | -0.255428 | -3.461906 | -0.477297 |
| 1  | -1.030933 | -3.168220 | -1.069745 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -0.289411 | -4.475653 | -0.415668 |
| 1 | 0.608947  | -3.210814 | -0.964136 |
| 7 | -3.061265 | -1.887782 | -1.018305 |
| 1 | -3.784563 | -1.180548 | -1.146104 |
| 1 | -2.824880 | -1.895795 | -0.024302 |
| 1 | -3.497778 | -2.780913 | -1.232224 |
| 7 | -3.940858 | 0.257754  | 1.328250  |
| 1 | -3.602436 | -0.649605 | 1.651271  |
| 1 | -4.544714 | 0.110029  | 0.518166  |
| 1 | -4.506669 | 0.665928  | 2.066200  |
| 7 | -0.357852 | -0.392542 | -1.419402 |
| 1 | 0.395648  | -1.067863 | -1.282175 |
| 1 | -0.103384 | 0.142365  | -2.246871 |
| 1 | -1.210809 | -0.924503 | -1.617445 |
| 7 | 2.465372  | -2.200017 | -1.508622 |
| 1 | 2.847108  | -2.974064 | -2.046885 |
| 1 | 3.085636  | -2.059327 | -0.712015 |
| 1 | 2.543824  | -1.362392 | -2.093179 |
| 7 | 4.824724  | -1.562066 | 0.844265  |
| 1 | 5.173081  | -2.517253 | 0.883393  |
| 1 | 5.127569  | -1.115470 | 1.706777  |
| 1 | 5.334807  | -1.105903 | 0.091314  |
| 7 | 2.471274  | 0.480255  | -3.236644 |
| 1 | 3.390507  | 0.850106  | -3.464436 |
| 1 | 1.868586  | 1.279055  | -3.014273 |
| 1 | 2.115850  | 0.065552  | -4.094763 |
| 7 | -0.896952 | 4.126091  | 0.557899  |
| 1 | 0.127379  | 4.166365  | 0.619921  |
| 1 | -1.273900 | 4.620722  | 1.362097  |
| 1 | -1.178808 | 4.655401  | -0.262407 |
| 7 | 2.181495  | 3.710333  | 0.778489  |
| 1 | 2.365345  | 2.707450  | 0.669933  |
| 1 | 2.466335  | 3.982160  | 1.715612  |
| 1 | 2.802064  | 4.204539  | 0.142768  |
| 7 | 2.273032  | 0.644470  | 0.131759  |
| 1 | 1.410953  | 0.138340  | 0.329788  |
| 1 | 3.016389  | 0.072204  | 0.531716  |
| 1 | 2.388857  | 0.593195  | -0.882213 |
| 7 | -5.836748 | -0.043843 | -1.320083 |
| 1 | -5.661415 | -0.041549 | -2.321695 |
| 1 | -6.321767 | 0.826406  | -1.116543 |
| 1 | -6.502019 | -0.792380 | -1.144116 |
| 7 | 0.615425  | 2.640592  | -1.976794 |
| 1 | -0.396667 | 2.582508  | -2.056687 |
| 1 | 0.866738  | 3.601840  | -2.194519 |
| 1 | 0.840972  | 2.502059  | -0.991854 |

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Cartesian coordinates of : BDC16

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.101290 | -0.010292 | 0.384823  |
| 1  | 0.868232  | -0.361379 | 0.630676  |
| 1  | 0.023718  | 0.998149  | 0.169250  |
| 1  | -0.507308 | -0.528552 | -0.423436 |
| 1  | -0.771733 | -0.155047 | 1.173033  |
| 7  | -1.631819 | -1.593944 | -1.534552 |
| 1  | -1.243317 | -2.505077 | -1.761327 |
| 1  | -2.501837 | -1.751568 | -1.009832 |
| 1  | -1.885622 | -1.158914 | -2.417011 |
| 7  | 2.608898  | -0.534595 | 0.978719  |
| 1  | 2.834050  | -0.742453 | 1.947727  |
| 1  | 3.095209  | -1.234159 | 0.402082  |
| 1  | 3.013411  | 0.379252  | 0.766703  |
| 7  | -2.209683 | -0.782402 | 2.209593  |
| 1  | -3.052527 | -0.210799 | 2.084709  |
| 1  | -2.078001 | -0.926382 | 3.206465  |
| 1  | -2.417575 | -1.689045 | 1.797028  |
| 7  | -7.271403 | -0.352706 | 0.366106  |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | -7.610341  | -1.070774 | 1.000630  |
| 1 | -6.986142  | -0.830719 | -0.486433 |
| 1 | -8.066192  | 0.252409  | 0.144913  |
| 7 | -4.823072  | 0.932127  | 1.727819  |
| 1 | -4.522825  | 1.762631  | 1.224531  |
| 1 | -5.696642  | 0.612449  | 1.288027  |
| 1 | -5.060966  | 1.237455  | 2.667938  |
| 7 | 0.901574   | 2.714155  | -0.058101 |
| 1 | 0.805161   | 3.159543  | -0.966339 |
| 1 | 0.648052   | 3.412357  | 0.635360  |
| 1 | 1.899034   | 2.515685  | 0.068090  |
| 7 | 4.100519   | -2.684553 | -0.687860 |
| 1 | 4.932411   | -2.976709 | -0.161570 |
| 1 | 3.532673   | -3.515009 | -0.830009 |
| 1 | 4.416488   | -2.392865 | -1.608325 |
| 7 | 6.613328   | -3.581914 | 0.949804  |
| 1 | 7.276588   | -2.825647 | 1.091181  |
| 1 | 7.119445   | -4.346247 | 0.494444  |
| 1 | 6.346454   | -3.908355 | 1.874032  |
| 7 | 8.192256   | -5.965025 | -0.447880 |
| 1 | 7.599592   | -6.780251 | -0.571536 |
| 1 | 8.996296   | -6.261252 | 0.097130  |
| 1 | 8.535199   | -5.704610 | -1.367492 |
| 7 | -9.769711  | 1.574731  | -0.125363 |
| 1 | -9.900421  | 2.070907  | 0.751190  |
| 1 | -10.643619 | 1.099654  | -0.329967 |
| 1 | -9.637961  | 2.277976  | -0.845937 |
| 7 | 4.064233   | 2.309850  | 0.172487  |
| 1 | 4.031959   | 3.268967  | -0.197573 |
| 1 | 4.614852   | 1.759695  | -0.482063 |
| 1 | 4.599727   | 2.346122  | 1.036063  |
| 7 | -4.320705  | -1.942289 | 0.033238  |
| 1 | -5.021391  | -1.976930 | -0.709472 |
| 1 | -4.525493  | -1.107576 | 0.583635  |
| 1 | -4.507866  | -2.739990 | 0.635680  |
| 7 | 3.763244   | 5.193194  | -0.935435 |
| 1 | 3.564797   | 5.223356  | -1.931514 |
| 1 | 4.625701   | 5.726040  | -0.787057 |
| 1 | 3.015361   | 5.704682  | -0.475710 |
| 7 | -6.537152  | -2.166700 | -2.385978 |
| 1 | -7.396446  | -2.681844 | -2.214662 |
| 1 | -5.933346  | -2.780294 | -2.926518 |
| 1 | -6.777828  | -1.388006 | -2.993122 |
| 7 | 6.433423   | 6.839148  | -0.495233 |
| 1 | 7.232436   | 6.359615  | -0.899009 |
| 1 | 6.641580   | 6.985119  | 0.488009  |
| 1 | 6.388489   | 7.756909  | -0.927931 |

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Cartesian coordinates of : BC16

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.243182  | 0.914371  | 0.145682  |
| 1  | 0.130849  | 0.149445  | 0.847403  |
| 1  | 1.253419  | 0.993196  | -0.138917 |
| 1  | -0.337514 | 0.618791  | -0.667991 |
| 1  | -0.093906 | 1.826486  | 0.535934  |
| 7  | -1.401054 | -0.463674 | -1.826795 |
| 1  | -1.265417 | -0.387678 | -2.830693 |
| 1  | -1.142607 | -1.410411 | -1.558035 |
| 1  | -2.405396 | -0.379161 | -1.642061 |
| 7  | -0.323452 | -1.456317 | 1.744445  |
| 1  | -1.076196 | -1.896573 | 1.202791  |
| 1  | 0.446709  | -2.117689 | 1.790367  |
| 1  | -0.662894 | -1.340501 | 2.695123  |
| 7  | -0.644683 | 3.462093  | 1.240105  |
| 1  | -0.442551 | 4.228133  | 0.582331  |
| 1  | -0.171289 | 3.687129  | 2.111172  |
| 1  | -1.640641 | 3.497990  | 1.440051  |

|   |            |           |           |
|---|------------|-----------|-----------|
| 7 | -2.735810  | -2.685101 | 0.126910  |
| 1 | -3.308464  | -3.079945 | 0.868471  |
| 1 | -2.614225  | -3.426502 | -0.558191 |
| 1 | -3.304866  | -1.961400 | -0.315729 |
| 7 | -0.038486  | 5.754789  | -0.736533 |
| 1 | -0.645655  | 5.729580  | -1.550829 |
| 1 | -0.167506  | 6.669548  | -0.293972 |
| 1 | 0.914211   | 5.726319  | -1.088382 |
| 7 | 3.022169   | 1.081641  | -0.604970 |
| 1 | 3.176155   | 1.097905  | -1.609796 |
| 1 | 3.491587   | 1.903235  | -0.233080 |
| 1 | 3.528040   | 0.260110  | -0.239879 |
| 7 | 9.358047   | -3.063095 | 0.548501  |
| 1 | 10.339832  | -2.930021 | 0.292274  |
| 1 | 9.314435   | -3.107380 | 1.562343  |
| 1 | 9.079234   | -3.977999 | 0.206457  |
| 7 | 4.612695   | -1.313527 | 0.448278  |
| 1 | 5.570105   | -1.146660 | 0.110612  |
| 1 | 4.336255   | -2.229912 | 0.107222  |
| 1 | 4.666048   | -1.388556 | 1.460273  |
| 7 | -4.532138  | -0.295643 | -1.227925 |
| 1 | -4.907653  | -0.253962 | -2.171990 |
| 1 | -4.616229  | 0.642753  | -0.845944 |
| 1 | -5.168656  | -0.895569 | -0.685409 |
| 7 | 7.496364   | -0.811508 | -0.575072 |
| 1 | 7.571160   | -0.834021 | -1.588019 |
| 1 | 8.115659   | -1.544745 | -0.210487 |
| 1 | 7.882272   | 0.080150  | -0.278226 |
| 7 | -6.315860  | -2.243071 | 0.370090  |
| 1 | -6.191004  | -3.216843 | 0.106951  |
| 1 | -7.271260  | -1.981124 | 0.094211  |
| 1 | -6.284504  | -2.211040 | 1.385401  |
| 7 | -0.425803  | 8.602082  | 0.605672  |
| 1 | -1.382537  | 8.757005  | 0.909118  |
| 1 | -0.197741  | 9.346729  | -0.046316 |
| 1 | 0.167140   | 8.729724  | 1.420241  |
| 7 | -9.178189  | -1.408847 | -0.513369 |
| 1 | -9.899213  | -2.053115 | -0.176723 |
| 1 | -9.258556  | -1.373427 | -1.525495 |
| 1 | -9.421829  | -0.483323 | -0.172569 |
| 7 | 12.404097  | -2.635951 | -0.270703 |
| 1 | 13.005464  | -3.404570 | 0.009715  |
| 1 | 12.785147  | -1.791614 | 0.145161  |
| 1 | 12.493265  | -2.538624 | -1.277493 |
| 7 | -11.436729 | -3.394418 | 0.514025  |
| 1 | -11.267044 | -4.349591 | 0.213915  |
| 1 | -12.352392 | -3.130619 | 0.162840  |
| 1 | -11.499701 | -3.408420 | 1.527464  |

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Cartesian coordinates of : BL16

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.029332 | -0.335838 | 0.789265  |
| 1  | -0.017920 | 0.654165  | 1.179407  |
| 1  | -0.906575 | -0.493141 | 0.206428  |
| 1  | 0.845493  | -0.509294 | 0.206005  |
| 1  | -0.035913 | -0.994926 | 1.565179  |
| 7  | 2.323752  | -0.825244 | -0.687358 |
| 1  | 2.854639  | 0.022638  | -0.869879 |
| 1  | 2.935240  | -1.452921 | -0.139027 |
| 1  | 2.177050  | -1.269485 | -1.590109 |
| 7  | 0.016499  | 2.304134  | 1.805913  |
| 1  | 0.722600  | 2.454221  | 2.522227  |
| 1  | 0.227656  | 2.960985  | 1.036160  |
| 1  | -0.866403 | 2.604469  | 2.211596  |
| 7  | 11.085260 | -5.924320 | -0.836865 |
| 1  | 11.799970 | -6.351201 | -0.255415 |
| 1  | 11.538092 | -5.195958 | -1.380457 |

|   |            |           |           |
|---|------------|-----------|-----------|
| 1 | 10.771124  | -6.633307 | -1.492394 |
| 7 | 4.119249   | -2.677543 | 0.910105  |
| 1 | 3.716577   | -3.577835 | 1.155477  |
| 1 | 4.492562   | -2.288800 | 1.771769  |
| 1 | 4.924369   | -2.869452 | 0.298015  |
| 7 | -11.116918 | -5.908885 | -0.893391 |
| 1 | -10.781569 | -6.732338 | -1.383836 |
| 1 | -11.905818 | -6.201154 | -0.324751 |
| 1 | -11.475725 | -5.269475 | -1.595880 |
| 7 | -2.389718  | -0.800009 | -0.690327 |
| 1 | -2.929964  | 0.043406  | -0.865761 |
| 1 | -2.239267  | -1.235006 | -1.597003 |
| 1 | -2.994673  | -1.438708 | -0.147488 |
| 7 | -8.816293  | -4.530653 | 0.819608  |
| 1 | -9.555144  | -4.978270 | 0.270820  |
| 1 | -8.433639  | -5.236607 | 1.441725  |
| 1 | -9.261303  | -3.834547 | 1.410580  |
| 7 | -4.168223  | -2.684755 | 0.887991  |
| 1 | -4.963583  | -2.884691 | 0.265767  |
| 1 | -4.556462  | -2.304428 | 1.746805  |
| 1 | -3.756145  | -3.580477 | 1.134415  |
| 7 | 6.550404   | -3.265947 | -0.908787 |
| 1 | 6.994384   | -2.435816 | -1.290747 |
| 1 | 6.336620   | -3.867001 | -1.699499 |
| 1 | 7.255577   | -3.752030 | -0.342226 |
| 7 | -6.568918  | -3.289443 | -0.965065 |
| 1 | -6.956036  | -2.469765 | -1.423744 |
| 1 | -7.316974  | -3.696160 | -0.391003 |
| 1 | -6.360544  | -3.958539 | -1.700674 |
| 7 | 8.665281   | -4.742587 | 0.858379  |
| 1 | 9.063996   | -4.124939 | 1.559380  |
| 1 | 9.443363   | -5.125717 | 0.315022  |
| 1 | 8.240440   | -5.515692 | 1.362011  |
| 7 | 0.593078   | 4.299098  | -0.407564 |
| 1 | 1.577962   | 4.475064  | -0.586091 |
| 1 | 0.191148   | 5.182604  | -0.065222 |
| 1 | 0.168897   | 4.111472  | -1.311684 |
| 7 | -0.582518  | 6.963159  | 0.640128  |
| 1 | -0.211519  | 7.723322  | 0.057743  |
| 1 | -0.317688  | 7.166203  | 1.599749  |
| 1 | -1.595797  | 7.026559  | 0.602272  |
| 7 | 0.558763   | 9.252377  | -1.158064 |
| 1 | 0.213278   | 9.178792  | -2.110481 |
| 1 | 1.572306   | 9.215744  | -1.214345 |
| 1 | 0.307740   | 10.183726 | -0.815937 |
| 7 | -0.232007  | 12.142294 | -0.086797 |
| 1 | 0.230861   | 12.354017 | 0.791853  |
| 1 | -1.231545  | 12.205899 | 0.080423  |
| 1 | 0.009756   | 12.883532 | -0.737372 |

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Cartesian coordinates of : P\_NH3\_N16\_8.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | 0.029227  | -0.058959 | 1.334630  |
| 1  | 0.899386  | -0.230417 | 1.880259  |
| 1  | 0.253652  | 0.355527  | 0.384766  |
| 1  | -0.505897 | -0.943699 | 1.210058  |
| 1  | -0.600950 | 0.645538  | 1.778108  |
| 7  | -1.509755 | -2.423779 | 0.602190  |
| 1  | -0.657083 | -2.860305 | 0.247117  |
| 1  | -2.093538 | -3.143094 | 1.018586  |
| 1  | -2.015981 | -2.025388 | -0.188847 |
| 7  | 2.564134  | -0.611664 | 2.769218  |
| 1  | 2.472178  | -1.401209 | 3.404491  |
| 1  | 3.352352  | -0.816574 | 2.137385  |
| 1  | 2.845546  | 0.175554  | 3.349376  |
| 7  | -2.004102 | 1.902050  | 1.805885  |
| 1  | -2.876010 | 1.372465  | 1.791891  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.940335 | 2.391729  | 0.911647  |
| 1 | -2.077368 | 2.603122  | 2.537191  |
| 7 | -4.621677 | -2.486861 | -0.760688 |
| 1 | -5.567679 | -2.403119 | -1.122620 |
| 1 | -4.392187 | -3.476449 | -0.787810 |
| 1 | -4.002393 | -2.013419 | -1.416239 |
| 7 | 1.609464  | -2.615994 | -0.020472 |
| 1 | 1.861718  | -2.326708 | 0.922825  |
| 1 | 1.954598  | -3.566841 | -0.128616 |
| 1 | 2.164327  | -2.028869 | -0.651126 |
| 7 | 0.413710  | 1.342143  | -1.097649 |
| 1 | 1.367697  | 1.702611  | -1.063909 |
| 1 | 0.323897  | 0.741452  | -1.918423 |
| 1 | -0.236292 | 2.126000  | -1.179482 |
| 7 | -2.620399 | 0.004071  | -1.090022 |
| 1 | -3.185171 | 0.527919  | -1.756481 |
| 1 | -3.161224 | 0.004078  | -0.223104 |
| 1 | -1.815301 | 0.602710  | -0.902170 |
| 7 | -2.258421 | 3.268005  | -1.171872 |
| 1 | -2.260684 | 3.242734  | -2.189204 |
| 1 | -2.189307 | 4.251950  | -0.923163 |
| 1 | -3.182750 | 2.945076  | -0.862980 |
| 7 | -4.039867 | -0.646801 | 1.701658  |
| 1 | -4.650382 | -0.637153 | 2.514957  |
| 1 | -3.140656 | -1.011676 | 2.014327  |
| 1 | -4.409129 | -1.348309 | 1.049619  |
| 7 | -0.137697 | -1.408510 | -2.519935 |
| 1 | 0.206297  | -1.969365 | -1.739717 |
| 1 | -0.143427 | -2.001885 | -3.344718 |
| 1 | -1.105741 | -1.168801 | -2.305191 |
| 7 | 3.314479  | 1.700420  | 0.110083  |
| 1 | 3.050699  | 0.972976  | 0.772602  |
| 1 | 3.083484  | 2.594091  | 0.536333  |
| 1 | 4.333142  | 1.661648  | 0.035146  |
| 7 | 4.667093  | -1.087076 | 0.593999  |
| 1 | 5.321197  | -0.312936 | 0.480042  |
| 1 | 4.171716  | -1.182838 | -0.294302 |
| 1 | 5.218625  | -1.930039 | 0.727768  |
| 7 | 6.571824  | 1.537504  | -0.222974 |
| 1 | 7.015431  | 0.975089  | -0.944611 |
| 1 | 7.195374  | 1.524797  | 0.580092  |
| 1 | 6.574157  | 2.493946  | -0.568878 |
| 7 | 2.930749  | -0.589274 | -2.067741 |
| 1 | 2.001981  | -0.639920 | -2.489715 |
| 1 | 3.607122  | -0.683518 | -2.820273 |
| 1 | 3.038074  | 0.346035  | -1.672068 |
| 7 | -4.951030 | 2.138634  | 0.088445  |
| 1 | -5.251445 | 2.852301  | 0.747552  |
| 1 | -4.821620 | 1.276623  | 0.620492  |
| 1 | -5.734232 | 1.989195  | -0.542258 |

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Cartesian coordinates of : P\_NH3\_N16\_15.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.122140 | 0.048938  | -0.197181 |
| 1  | 0.200191  | 0.312219  | 0.754372  |
| 1  | -0.773844 | 0.783085  | -0.579270 |
| 1  | 0.747065  | -0.024444 | -0.784966 |
| 1  | -0.611104 | -0.871020 | -0.166977 |
| 7  | 2.412013  | -0.073015 | -1.565507 |
| 1  | 2.441686  | -0.160530 | -2.578207 |
| 1  | 2.926732  | 0.779198  | -1.323370 |
| 1  | 2.943958  | -0.859744 | -1.193202 |
| 7  | 1.319501  | 0.938717  | 2.227165  |
| 1  | 2.261350  | 0.657346  | 1.931545  |
| 1  | 1.296337  | 1.954987  | 2.232968  |
| 1  | 1.199929  | 0.646697  | 3.193300  |
| 7  | -1.356699 | -2.628278 | 0.016627  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.382699 | -3.259255 | -0.780512 |
| 1 | -2.223659 | -2.777067 | 0.550487  |
| 1 | -0.567998 | -2.922662 | 0.591312  |
| 7 | 4.111402  | 0.017070  | 1.096640  |
| 1 | 4.766652  | 0.102030  | 1.868996  |
| 1 | 4.247592  | 0.829735  | 0.494183  |
| 1 | 4.387507  | -0.808050 | 0.554044  |
| 7 | 4.082175  | 2.612472  | -0.961769 |
| 1 | 3.447231  | 3.361665  | -0.700194 |
| 1 | 4.939943  | 2.737922  | -0.414267 |
| 1 | 4.330788  | 2.776209  | -1.934069 |
| 7 | -2.088445 | 1.836355  | -1.282940 |
| 1 | -2.516436 | 2.566732  | -0.711456 |
| 1 | -1.890279 | 2.250803  | -2.189496 |
| 1 | -2.788003 | 1.099917  | -1.427341 |
| 7 | 1.598021  | -3.099175 | -1.638702 |
| 1 | 1.121308  | -2.560059 | -2.355290 |
| 1 | 1.283620  | -4.061090 | -1.726094 |
| 1 | 1.301427  | -2.745108 | -0.726993 |
| 7 | -3.814157 | -0.739274 | -1.281936 |
| 1 | -4.278190 | -1.245829 | -2.031004 |
| 1 | -4.454999 | -0.720910 | -0.486684 |
| 1 | -3.017867 | -1.304980 | -0.991918 |
| 7 | 4.495360  | -2.565591 | -0.690172 |
| 1 | 5.197555  | -2.415636 | -1.410009 |
| 1 | 3.657415  | -2.929261 | -1.155426 |
| 1 | 4.855821  | -3.306668 | -0.094827 |
| 7 | -4.129746 | -2.936400 | 1.344336  |
| 1 | -4.656076 | -3.626358 | 0.814923  |
| 1 | -4.666171 | -2.065800 | 1.309797  |
| 1 | -4.131766 | -3.254821 | 2.309367  |
| 7 | -5.910414 | -0.251429 | 1.195730  |
| 1 | -6.853542 | -0.625919 | 1.131505  |
| 1 | -5.885461 | 0.594626  | 0.614647  |
| 1 | -5.788549 | 0.045955  | 2.160197  |
| 7 | -3.527103 | 4.258911  | 0.427553  |
| 1 | -4.114736 | 4.029675  | 1.224931  |
| 1 | -3.981633 | 5.025349  | -0.061826 |
| 1 | -2.660424 | 4.633422  | 0.803822  |
| 7 | -5.512208 | 1.985066  | -0.924881 |
| 1 | -4.807971 | 2.686263  | -0.702059 |
| 1 | -6.285098 | 2.458491  | -1.383003 |
| 1 | -5.089700 | 1.352481  | -1.600841 |
| 7 | 6.710774  | 2.636374  | 0.751408  |
| 1 | 6.622686  | 2.825442  | 1.745678  |
| 1 | 7.368406  | 3.318307  | 0.383726  |
| 1 | 7.151439  | 1.725389  | 0.659941  |
| 7 | 1.616623  | -2.153270 | 1.363720  |
| 1 | 2.322084  | -1.438768 | 1.169945  |
| 1 | 2.127310  | -2.971525 | 1.687785  |
| 1 | 1.085470  | -1.810741 | 2.161193  |

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Cartesian coordinates of : P\_NH3\_N16\_16.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.192990 | 1.471118  | -0.087531 |
| 1  | -0.134549 | 1.294725  | 0.934266  |
| 1  | 0.779944  | 1.736813  | -0.391453 |
| 1  | -0.485931 | 0.600107  | -0.575360 |
| 1  | -0.914590 | 2.194539  | -0.336068 |
| 7  | -1.421939 | -0.626977 | -1.727019 |
| 1  | -2.074688 | -1.233444 | -1.220264 |
| 1  | -2.006487 | 0.064665  | -2.194414 |
| 1  | -0.975859 | -1.181735 | -2.452117 |
| 7  | 0.740106  | 0.626831  | 2.516787  |
| 1  | 1.591873  | 1.158169  | 2.676751  |
| 1  | 0.363577  | 0.364531  | 3.421627  |
| 1  | 1.004912  | -0.217878 | 1.999889  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | -2.403267 | 3.046731  | -0.990703 |
| 1 | -2.244272 | 3.609026  | -1.822188 |
| 1 | -2.876004 | 3.649783  | -0.311294 |
| 1 | -3.050787 | 2.298853  | -1.253881 |
| 7 | -4.374307 | 0.555869  | -1.654066 |
| 1 | -4.650140 | 0.305931  | -2.600219 |
| 1 | -5.196044 | 0.965064  | -1.217279 |
| 1 | -4.185547 | -0.318213 | -1.160806 |
| 7 | 6.638675  | -0.981570 | -0.017259 |
| 1 | 7.267120  | -0.599176 | 0.684656  |
| 1 | 7.086232  | -1.829958 | -0.379966 |
| 1 | 6.615861  | -0.308540 | -0.778774 |
| 7 | 2.580631  | 2.017157  | -0.610212 |
| 1 | 2.756649  | 3.023003  | -0.522889 |
| 1 | 3.103995  | 1.542090  | 0.134703  |
| 1 | 2.996582  | 1.729677  | -1.492557 |
| 7 | 4.096395  | -2.950040 | 0.431641  |
| 1 | 4.902114  | -2.336743 | 0.293745  |
| 1 | 4.179157  | -3.347636 | 1.363104  |
| 1 | 4.185956  | -3.720632 | -0.224128 |
| 7 | 1.496648  | -1.206890 | 0.162470  |
| 1 | 1.855755  | -0.423732 | -0.381199 |
| 1 | 0.682562  | -1.561773 | -0.332538 |
| 1 | 2.225071  | -1.927067 | 0.155182  |
| 7 | -3.581582 | -2.272521 | -0.072558 |
| 1 | -3.206881 | -2.203716 | 0.870095  |
| 1 | -3.417781 | -3.228752 | -0.376804 |
| 1 | -4.600763 | -2.157493 | 0.000587  |
| 7 | 3.993027  | 0.170073  | 1.524940  |
| 1 | 4.298054  | 0.442106  | 2.455291  |
| 1 | 4.803869  | -0.233694 | 1.052356  |
| 1 | 3.318301  | -0.584758 | 1.633554  |
| 7 | -6.633072 | -1.747570 | -0.039751 |
| 1 | -6.945636 | -1.000813 | 0.574510  |
| 1 | -7.125278 | -2.597584 | 0.253219  |
| 1 | -6.968617 | -1.517320 | -0.971007 |
| 7 | 7.901624  | -3.691397 | -1.006350 |
| 1 | 8.911481  | -3.615895 | -1.087247 |
| 1 | 7.559222  | -4.021839 | -1.903667 |
| 1 | 7.714117  | -4.424170 | -0.328375 |
| 7 | -8.167503 | -4.361474 | 0.865245  |
| 1 | -9.162610 | -4.189722 | 0.974495  |
| 1 | -7.827680 | -4.710938 | 1.756242  |
| 1 | -8.070194 | -5.117883 | 0.194487  |
| 7 | -3.805349 | 5.003828  | 1.095413  |
| 1 | -4.730281 | 5.296303  | 0.794648  |
| 1 | -3.249822 | 5.847299  | 1.202467  |
| 1 | -3.907824 | 4.598432  | 2.020865  |
| 7 | 3.148631  | 5.141303  | -0.394630 |
| 1 | 2.990906  | 5.626673  | -1.272673 |
| 1 | 4.120738  | 5.293250  | -0.142680 |
| 1 | 2.584108  | 5.608767  | 0.308189  |

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Cartesian coordinates of : P\_NH3\_N16\_4.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -0.903598 | -1.490295 | -0.525625 |
| 1  | -1.474410 | -0.717365 | -0.094622 |
| 1  | -1.436126 | -2.034354 | -1.236513 |
| 1  | -0.077946 | -1.009111 | -0.933163 |
| 1  | -0.517985 | -2.099075 | 0.245360  |
| 7  | 1.446597  | 0.174118  | -0.675399 |
| 1  | 2.317719  | 0.298600  | -1.195745 |
| 1  | 1.138459  | 1.107227  | -0.392914 |
| 1  | 1.732636  | -0.292951 | 0.188311  |
| 7  | -1.930561 | 0.917286  | 0.596548  |
| 1  | -1.777003 | 1.554965  | -0.184847 |
| 1  | -2.854331 | 1.110827  | 1.002014  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.233172 | 1.146985  | 1.300817  |
| 7 | 0.460231  | -2.797892 | 1.610561  |
| 1 | -0.029889 | -2.758492 | 2.500187  |
| 1 | 1.292181  | -2.208717 | 1.704277  |
| 1 | 0.772024  | -3.765542 | 1.486526  |
| 7 | -2.356094 | -3.023580 | -2.581315 |
| 1 | -2.408620 | -2.531982 | -3.469523 |
| 1 | -1.885471 | -3.904295 | -2.771863 |
| 1 | -3.318491 | -3.253043 | -2.309715 |
| 7 | 3.092863  | -0.909988 | 1.906468  |
| 1 | 3.173372  | 0.111044  | 1.897821  |
| 1 | 3.305492  | -1.225168 | 2.849426  |
| 1 | 3.841805  | -1.249472 | 1.306190  |
| 7 | 4.586950  | 0.164946  | -1.492618 |
| 1 | 5.073327  | 0.766980  | -2.151637 |
| 1 | 4.508340  | -0.741600 | -1.946095 |
| 1 | 5.204533  | 0.045625  | -0.683237 |
| 7 | 0.485331  | 3.253122  | 0.142734  |
| 1 | 0.991923  | 4.085752  | -0.147195 |
| 1 | -0.111094 | 3.535958  | 0.915754  |
| 1 | -0.129050 | 2.993085  | -0.634569 |
| 7 | -4.738343 | 1.476192  | 1.834054  |
| 1 | -5.149851 | 0.620877  | 2.196431  |
| 1 | -5.388332 | 1.838492  | 1.142231  |
| 1 | -4.720397 | 2.148757  | 2.605804  |
| 7 | -5.308157 | -3.765718 | -1.799588 |
| 1 | -5.348014 | -4.449897 | -1.049877 |
| 1 | -5.799252 | -4.168807 | -2.592278 |
| 1 | -5.849617 | -2.962392 | -1.494486 |
| 7 | -0.907113 | 1.859411  | -2.300821 |
| 1 | -0.240310 | 1.089690  | -2.265348 |
| 1 | -0.606460 | 2.497786  | -3.044044 |
| 1 | -1.797999 | 1.468490  | -2.596146 |
| 7 | 1.386202  | -5.833875 | 1.332441  |
| 1 | 1.897467  | -6.041354 | 0.479840  |
| 1 | 0.596348  | -6.471474 | 1.366079  |
| 1 | 1.994483  | -6.077849 | 2.108431  |
| 7 | 3.465933  | 2.070977  | 0.985689  |
| 1 | 2.494704  | 2.378216  | 0.910742  |
| 1 | 3.721276  | 1.696530  | 0.070516  |
| 1 | 4.024682  | 2.904987  | 1.146054  |
| 7 | -4.816077 | 3.557977  | 4.241072  |
| 1 | -4.548523 | 4.497012  | 3.961900  |
| 1 | -4.223068 | 3.300984  | 5.024361  |
| 1 | -5.766404 | 3.614249  | 4.595173  |
| 7 | 6.105002  | 0.298979  | 1.250050  |
| 1 | 6.354658  | -0.437473 | 1.903592  |
| 1 | 5.355238  | 0.844894  | 1.672894  |
| 1 | 6.919631  | 0.901045  | 1.169888  |
| 7 | -0.073955 | 3.940106  | -4.543049 |
| 1 | 0.918846  | 4.149842  | -4.585200 |
| 1 | -0.554820 | 4.817740  | -4.369186 |
| 1 | -0.348980 | 3.631411  | -5.470831 |

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Cartesian coordinates of : P\_NH3\_N16\_13.log

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Atomic number (AN) and Cartesian coordinates

| AN | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| 7  | -1.470404 | 0.879964  | -0.060385 |
| 1  | -1.708051 | 0.554594  | 0.893959  |
| 1  | -1.677231 | 0.045306  | -0.659025 |
| 1  | -2.053702 | 1.699541  | -0.328244 |
| 1  | -0.432917 | 1.129942  | -0.099914 |
| 7  | 0.504660  | 0.676779  | 3.103064  |
| 1  | 0.789137  | 0.124801  | 3.907374  |
| 1  | -0.492536 | 0.511044  | 2.967821  |
| 1  | 0.625581  | 1.652773  | 3.358424  |
| 7  | 0.692766  | -1.572389 | 0.725172  |
| 1  | 1.435129  | -2.271216 | 0.743145  |

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|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 0.874861  | -1.038974 | -0.124396 |
| 1 | 0.884274  | -0.916381 | 1.485230  |
| 7 | -2.081440 | -0.923387 | 2.179107  |
| 1 | -1.316376 | -1.496751 | 1.815377  |
| 1 | -2.108676 | -1.039270 | 3.194574  |
| 1 | -2.945174 | -1.306246 | 1.793329  |
| 7 | -3.060766 | 3.274582  | -0.754362 |
| 1 | -3.882502 | 3.390971  | -0.167804 |
| 1 | -3.381999 | 3.289415  | -1.727966 |
| 1 | -2.489644 | 4.104252  | -0.618005 |
| 7 | 2.979342  | -0.815166 | -1.497779 |
| 1 | 3.059716  | -1.663612 | -0.931654 |
| 1 | 2.706142  | -1.102603 | -2.433116 |
| 1 | 3.910491  | -0.416336 | -1.576239 |
| 7 | -2.045056 | -1.764155 | -0.984819 |
| 1 | -1.241212 | -2.144989 | -0.483735 |
| 1 | -2.120531 | -2.235194 | -1.888476 |
| 1 | -2.874946 | -1.993580 | -0.438352 |
| 7 | 1.278508  | 1.488843  | 0.010525  |
| 1 | 1.535108  | 2.465179  | -0.168823 |
| 1 | 1.875780  | 0.885053  | -0.560018 |
| 1 | 1.490008  | 1.279838  | 0.986263  |
| 7 | -4.724943 | -2.506983 | 0.899558  |
| 1 | -4.519327 | -3.465715 | 1.166711  |
| 1 | -5.272136 | -2.550117 | 0.044212  |
| 1 | -5.339111 | -2.127478 | 1.614915  |
| 7 | -1.863425 | -0.912184 | 5.377326  |
| 1 | -1.177972 | -1.543992 | 5.780808  |
| 1 | -2.760084 | -1.154199 | 5.789201  |
| 1 | -1.635562 | 0.023288  | 5.701234  |
| 7 | -4.049450 | 3.371027  | -3.742616 |
| 1 | -4.438567 | 4.279018  | -3.978938 |
| 1 | -4.771036 | 2.681793  | -3.931473 |
| 1 | -3.292208 | 3.193618  | -4.395714 |
| 7 | -2.303368 | -3.275053 | -3.818321 |
| 1 | -3.220350 | -3.192216 | -4.246556 |
| 1 | -2.108891 | -4.267175 | -3.722943 |
| 1 | -1.631802 | -2.902367 | -4.482529 |
| 7 | 2.026020  | 4.517317  | -0.551424 |
| 1 | 1.355160  | 5.201777  | -0.214907 |
| 1 | 2.101795  | 4.657294  | -1.554849 |
| 1 | 2.932566  | 4.763230  | -0.144876 |
| 7 | 3.298686  | -3.605801 | 0.146028  |
| 1 | 3.622538  | -3.629809 | 1.109362  |
| 1 | 4.118061  | -3.781412 | -0.444220 |
| 1 | 2.677310  | -4.402118 | 0.031046  |
| 7 | 4.844033  | 5.329568  | 0.695961  |
| 1 | 5.349409  | 4.515435  | 1.031773  |
| 1 | 4.752359  | 5.967896  | 1.480401  |
| 1 | 5.436770  | 5.787092  | 0.009931  |
| 7 | 5.827278  | -4.053968 | -1.701250 |
| 1 | 6.633127  | -3.532250 | -1.369601 |
| 1 | 5.657799  | -3.760886 | -2.658711 |
| 1 | 6.102338  | -5.031223 | -1.734508 |

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