

# The importance of second shell effects in the simulation of hydrated Sr<sup>2+</sup> hydroxide complexes

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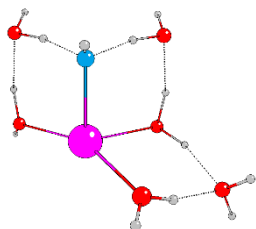
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**Electronic Supplementary Information**

## 1. Sr<sup>2+</sup> hydroxide complexes with a first solvation shell

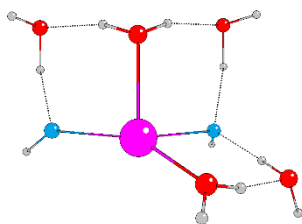
### 1.1. [Sr:3/3:1/0]<sup>+</sup>



SCF Energy = -565.5202782749

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -1.0146625 | 0.3581517  | 0.9151213  |
| O     | -2.2231815 | 2.0451591  | -0.5260129 |
| O     | -0.0092754 | -1.2080368 | -0.7874119 |
| H     | 0.1129081  | -2.1390636 | -0.4915350 |
| O     | 0.9177276  | 1.7201035  | 0.4985571  |
| H     | 1.4796036  | 2.0483014  | 1.2180043  |
| H     | -1.5583961 | 2.7463853  | -0.8092389 |
| H     | -2.8161167 | 1.8948750  | -1.2787512 |
| O     | -0.9217582 | -1.7681158 | 2.2997161  |
| H     | -1.5078826 | -2.0527914 | 3.0184674  |
| H     | -0.6300962 | -2.5903533 | 1.8298809  |
| H     | 0.8967938  | -0.8499622 | -1.0272138 |
| O     | -0.1539269 | 3.6818091  | -0.8548274 |
| H     | 0.2304243  | 3.7205796  | -1.7455344 |
| H     | 0.3837510  | 2.9730690  | -0.3440170 |
| O     | 2.2784639  | 0.1549078  | -1.0986030 |
| H     | 2.3903804  | 0.5814906  | -1.9634975 |
| H     | 1.8395273  | 0.8541223  | -0.4918838 |
| O     | 0.0245642  | -3.6728779 | 0.5752178  |
| H     | -0.5768696 | -4.3737283 | 0.2714038  |
| H     | 0.8580217  | -4.1240249 | 0.7921582  |

### 1.2. [Sr:2/3:2/0]

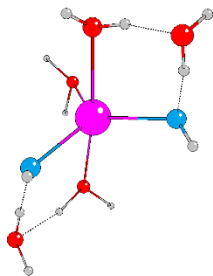


SCF Energy = -565.0525454927

| Atoms | X         | Y          | Z          |
|-------|-----------|------------|------------|
| Sr    | 0.9855686 | 0.1227192  | 0.6532514  |
| O     | 0.7458200 | -0.8569034 | -1.6972183 |

|   |            |            |            |
|---|------------|------------|------------|
| O | -2.1526233 | -1.0307045 | 2.5815495  |
| O | 2.2892479  | 1.8038174  | -0.3538040 |
| H | 2.6386869  | 2.6875374  | -0.1731057 |
| O | -1.4132661 | 0.5001230  | 0.6087061  |
| H | -0.2274446 | -0.7810566 | -1.9041400 |
| H | -1.9688738 | -0.3674865 | 1.8153944  |
| H | 1.2223594  | -0.1965651 | -2.2797107 |
| H | -2.4618886 | -0.4922782 | 3.3279928  |
| H | -1.7846754 | 1.3933844  | 0.6795297  |
| H | -0.5061869 | -1.4037286 | 2.7722822  |
| O | 0.4788105  | -1.5018340 | 2.5932409  |
| H | 0.9149313  | -1.5495606 | 3.4583896  |
| O | 2.1665332  | 1.1552656  | -2.8360999 |
| H | 3.0399874  | 0.8542272  | -3.1339755 |
| H | 2.2993690  | 1.4957740  | -1.8595106 |
| O | -1.9527979 | -0.4644969 | -1.7657674 |
| H | -2.4646488 | -1.2835985 | -1.6682628 |
| H | -1.8489088 | -0.0846356 | -0.8187418 |

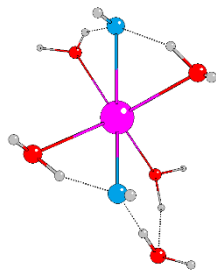
### 1.3. [Sr:3/2:2/0]



SCF Energy = -565.0482594933

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | 0.0272475  | -0.0213109 | 0.0044156  |
| O     | -1.3776535 | -0.3748927 | -2.1373551 |
| O     | -0.0409545 | 1.0456764  | 3.7447433  |
| O     | -0.1731479 | -2.5781278 | 0.5627575  |
| O     | 1.6381807  | 0.8318682  | -1.5368125 |
| H     | 2.2055731  | 1.6092475  | -1.4270337 |
| O     | -1.0579501 | 1.5169142  | 1.4652516  |
| H     | -2.2928515 | -0.0791072 | -2.2634767 |
| H     | -0.4926645 | 1.3508640  | 2.8404023  |
| H     | 0.1828323  | -2.5728254 | 1.4711013  |
| H     | -0.8343774 | 0.0476490  | -2.8761581 |
| H     | 0.5319676  | 1.7795607  | 4.0194838  |
| H     | -0.9612637 | -3.1445371 | 0.5917153  |
| H     | -1.2912418 | 2.4428139  | 1.3039967  |
| H     | 0.8673030  | -0.0991177 | 2.9388417  |
| O     | 1.2121453  | -0.7520094 | 2.2484224  |
| H     | 2.1714044  | -0.8133444 | 2.3803561  |
| O     | 0.3846471  | 0.7945675  | -3.7467621 |
| H     | 0.8166157  | 0.1658818  | -4.3470799 |
| H     | 0.9946073  | 0.8472649  | -2.8869547 |

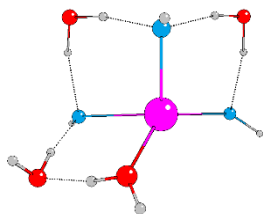
### 1.4. [Sr:4/1:2/0]



SCF Energy = -565.0474029244

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -0.0578182 | -0.0390574 | -0.3196584 |
| O     | 2.0981258  | 1.2673588  | -1.0417078 |
| O     | -0.5658777 | -1.6416636 | -2.3645605 |
| O     | 0.9975223  | -1.7514273 | 1.2512163  |
| O     | -2.5792132 | 0.3728610  | 0.2902036  |
| O     | -0.6320022 | 1.1295674  | 1.7906997  |
| H     | -0.4734953 | 2.0704905  | 1.9602644  |
| O     | 0.2168911  | 0.7778323  | -2.6982351 |
| H     | 1.4947147  | 1.2945773  | -1.8697043 |
| H     | -0.3669630 | -0.7332080 | -2.7886906 |
| H     | -2.0613084 | 0.8511373  | 1.0258002  |
| H     | 0.9229311  | -1.3801632 | 2.1857026  |
| H     | 2.2795609  | 2.1879029  | -0.7944249 |
| H     | -1.4507453 | -1.9037309 | -2.6639834 |
| H     | -3.1417429 | 1.0391604  | -0.1358923 |
| H     | 1.8658388  | -2.1788337 | 1.1869985  |
| H     | -0.3341079 | 1.4749485  | -3.0846895 |
| O     | 0.4287402  | -0.4693187 | 3.5129596  |
| H     | 1.1947862  | -0.0534548 | 3.9399552  |
| H     | 0.0068552  | 0.2619962  | 2.9110440  |

### 1.5. [Sr:1/3:3/0]<sup>-</sup>

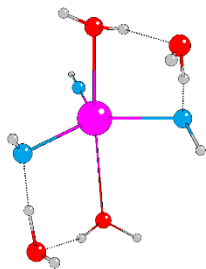


SCF Energy = -564.5743523453

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -0.5084375 | 0.1291068  | 0.1177550  |
| O     | 1.1276816  | -1.0017946 | -1.2942859 |
| O     | -1.4410567 | -1.0856256 | 1.9272683  |
| O     | 3.0836921  | 0.4863364  | -0.0339819 |
| O     | 0.0700532  | 0.4102964  | 3.6170642  |
| O     | 1.0028114  | 1.5792821  | 1.3248442  |
| H     | 0.9626764  | 2.5470080  | 1.2858860  |
| O     | -1.4345613 | 1.1215345  | -2.0852383 |
| H     | 0.4816544  | 0.9419545  | 2.8745318  |
| H     | 2.4075964  | 0.9814191  | 0.5213209  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 1.3047937  | -1.9546885 | -1.2843803 |
| H | -2.3637387 | -1.1976756 | 2.1991913  |
| H | -0.5555440 | -0.1928738 | 3.1087469  |
| H | 2.4967831  | -0.1195223 | -0.5673977 |
| H | -2.3468351 | 1.0191850  | -2.3993949 |
| H | -0.8414329 | 0.7108071  | -2.7906245 |
| O | 0.3569555  | -0.1551335 | -3.5845016 |
| H | 1.0370314  | 0.4327095  | -3.9508967 |
| H | 0.7565400  | -0.5471517 | -2.7006586 |

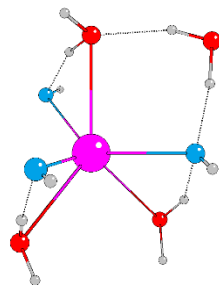
### 1.6. [Sr:2/2:3/0]<sup>-</sup>



SCF Energy = -564.5704310170

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | 0.4040985  | 0.9543843  | 0.0074525  |
| O     | -1.2349546 | 1.2333923  | 2.0596279  |
| O     | -1.4192575 | 0.3416765  | -1.5076018 |
| O     | 1.7827054  | -0.0830131 | -2.0045664 |
| H     | 2.4994459  | -0.7168478 | -1.8444104 |
| O     | 1.2244549  | -0.8068253 | 1.5033449  |
| H     | -1.1533640 | 0.3705673  | 2.5755166  |
| H     | -2.1845640 | 1.4083871  | 1.9693901  |
| H     | -2.2806612 | 0.0153813  | -1.2069464 |
| H     | 1.5982946  | -1.6434888 | 1.1887257  |
| O     | 1.2861452  | 3.0918496  | -0.0169072 |
| H     | 1.6415146  | 3.9903707  | -0.0244003 |
| O     | -0.5848737 | -1.0664530 | 3.2347302  |
| O     | -0.3347347 | -1.0904461 | -3.2714814 |
| H     | 0.2025570  | -1.0647125 | 2.5089581  |
| H     | -1.1813972 | -1.7884220 | 2.9797969  |
| H     | -0.4714413 | -2.0287131 | -3.0638871 |
| H     | 1.0925898  | -0.5749534 | -2.5521368 |
| H     | -0.8865578 | -0.5421339 | -2.5352051 |

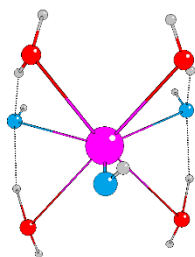
### 1.7. [Sr:3/1:3/0]<sup>-</sup>



SCF Energy = -564.5680311812

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -0.3120191 | 0.1631074  | 0.3893266  |
| O     | 2.4059789  | -0.1382495 | 0.7751749  |
| O     | -2.5908603 | 0.6539706  | 1.7569492  |
| O     | -1.4724435 | 1.2861537  | -1.7792222 |
| O     | -0.1089115 | -0.8709016 | -1.8615352 |
| H     | -0.5333192 | -1.7155053 | -2.0761963 |
| O     | -1.1029909 | -1.3512794 | 2.1293395  |
| H     | 2.7725427  | -0.5133406 | 1.5911379  |
| H     | -2.1923600 | -0.2719725 | 2.0317399  |
| H     | -1.0553977 | 0.3907927  | -2.0656756 |
| H     | 2.0797481  | 0.8500119  | 0.9868369  |
| H     | -3.4464722 | 0.4731666  | 1.3367150  |
| H     | -2.4268571 | 1.2081008  | -1.9355667 |
| H     | -1.4585926 | -2.2421157 | 1.9927014  |
| O     | 1.1519882  | 1.9924004  | 1.1218376  |
| H     | 1.4401983  | 2.7360433  | 0.5713645  |
| O     | 2.5673816  | -0.9628786 | -1.9502567 |
| H     | 2.7229438  | -0.7116232 | -1.0136421 |
| H     | 1.5594426  | -0.9758812 | -2.0010285 |

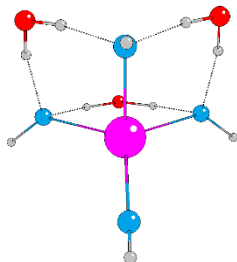
### 1.8. [Sr:4/0:3/0]<sup>-</sup>



SCF Energy = -564.5642657015

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -0.0086890 | -0.1880202 | 0.0185480  |
| O     | -2.5392055 | -0.2183494 | -1.0654659 |
| O     | -0.7704968 | 0.3230483  | 2.5822552  |
| O     | 0.5898404  | 0.1406091  | -2.6151284 |
| O     | 2.4616682  | 0.1162893  | 1.1239876  |
| O     | 1.7901349  | 1.5454131  | -0.8696742 |
| H     | 1.5696309  | 2.4822174  | -0.7537343 |
| O     | -1.8706440 | 1.5454843  | 0.6440866  |
| H     | -2.4703465 | 0.6266882  | -0.4854620 |
| H     | -1.2761045 | 0.9945110  | 1.9876697  |
| H     | 2.3764972  | 0.8438858  | 0.3985477  |
| H     | 1.1244531  | 0.8609636  | -2.1065250 |
| H     | -2.6597875 | 0.0843632  | -1.9790079 |
| H     | -0.2024230 | 0.8472717  | 3.1681040  |
| H     | 2.5655027  | 0.5813172  | 1.9688530  |
| H     | -0.0064706 | 0.6125678  | -3.2170459 |
| H     | -1.7129231 | 2.4783130  | 0.4350322  |
| O     | 0.1062153  | -2.5267029 | 0.0860344  |
| H     | -0.5029311 | -3.1778647 | -0.2923478 |

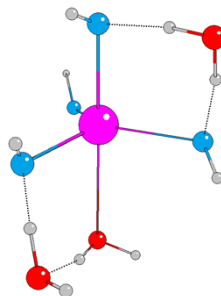
### 1.9. [Sr:0/3:4/0]<sup>2-</sup>



SCF Energy = -564.0962794625

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -0.7205792 | 0.8630581  | -0.0000024 |
| O     | -0.7646925 | -0.7464329 | -1.8475578 |
| O     | -0.7646750 | -0.7464501 | 1.8475800  |
| O     | 1.8576820  | -0.1927103 | -2.2838448 |
| O     | 1.8576817  | -0.1926918 | 2.2838287  |
| O     | 1.6946422  | 1.2690022  | -0.0000101 |
| H     | 2.1115052  | 2.1438574  | 0.0000036  |
| O     | -2.1769212 | 2.6585191  | -0.0000008 |
| H     | 1.9314803  | 0.3851511  | 1.4649402  |
| H     | 1.9315099  | 0.3851102  | -1.4649311 |
| H     | -1.3704718 | -0.7292746 | -2.6037266 |
| H     | -1.3704676 | -0.7292453 | 2.6037287  |
| H     | 0.8917476  | -0.4673685 | 2.2484917  |
| H     | 0.8917302  | -0.4672906 | -2.2484806 |
| H     | -2.7877394 | 3.4071792  | 0.0000024  |
| O     | -1.1467919 | -2.6967216 | 0.0000182  |
| H     | -1.0328544 | -2.0718179 | 0.7794294  |
| H     | -1.0327862 | -2.0718736 | -0.7794689 |

### 1.10. [Sr:1/2:4/0]<sup>2-</sup>

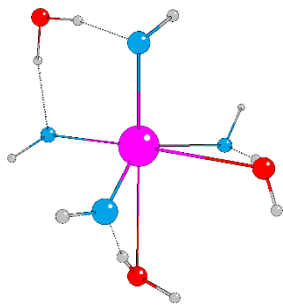


SCF Energy = -564.0898062481

| Atoms | X          | Y          | Z         |
|-------|------------|------------|-----------|
| O     | 0.2465132  | 1.5765462  | 0.1616909 |
| Sr    | -1.1889349 | 1.1260517  | 2.6524024 |
| O     | -3.1547345 | 0.4597531  | 1.5000989 |
| O     | 0.1388761  | 3.2410453  | 2.1896402 |
| O     | 0.3702982  | -0.7304999 | 2.8993688 |
| O     | -1.5388959 | 4.3496790  | 4.0398600 |
| O     | 1.9869741  | -0.4632008 | 0.9444904 |

|   |            |            |           |
|---|------------|------------|-----------|
| O | -2.0067106 | 1.8302196  | 4.8275378 |
| H | -2.9109376 | 1.7030315  | 5.1525069 |
| H | 0.9498000  | 0.9080817  | 0.3704143 |
| H | 0.3522325  | 2.3135908  | 0.8555807 |
| H | 1.0122824  | 3.3240584  | 2.6039309 |
| H | 0.8408056  | -0.9483016 | 3.7181806 |
| H | -3.2467444 | 0.2233441  | 0.5649951 |
| H | 1.3795203  | -0.6009994 | 1.7956701 |
| H | 2.8178799  | -0.0868646 | 1.2755471 |
| H | -1.7905241 | 3.4519522  | 4.4366462 |
| H | -0.8887345 | 4.0709494  | 3.3286845 |

### 1.11. [Sr:2/1:4/0]<sup>2-</sup>

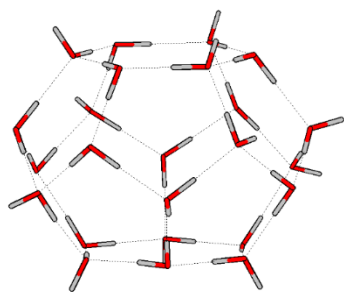


SCF Energy = -564.0857030233

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | 0.0523994  | 0.2408549  | -0.1192058 |
| O     | -0.6161094 | 2.8686058  | 0.8131879  |
| O     | -1.9366220 | 0.0385186  | -1.5069950 |
| O     | 1.6771265  | 0.3028245  | 2.2330066  |
| O     | 1.3250632  | -1.5358895 | -1.1896344 |
| O     | -0.6253761 | -0.7288134 | 2.0892682  |
| H     | -0.6233863 | -1.6841592 | 2.2550330  |
| O     | 1.1342728  | 2.3463260  | -0.9347160 |
| H     | 0.9302689  | 2.7314397  | -1.8008414 |
| H     | 0.1411070  | 2.8337570  | 0.0830985  |
| H     | 0.7419412  | -0.1645903 | 2.3544652  |
| H     | -0.1897953 | 3.1734615  | 1.6294818  |
| H     | -2.2522407 | 0.7843291  | -2.0399997 |
| H     | 1.5784691  | -2.3381994 | -0.7079323 |
| H     | 1.6530421  | 1.1030866  | 2.7806724  |
| O     | -0.7080466 | -1.8947746 | -2.9159708 |
| H     | 0.1075608  | -1.8761512 | -2.3192497 |
| H     | -1.2645970 | -1.1670472 | -2.4886131 |

## 2. W24 water cluster





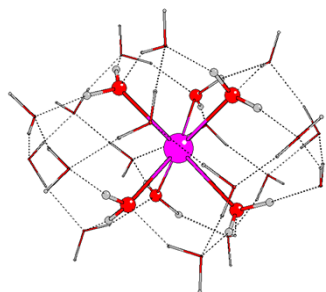
SCF Energy = -1835.6524726596

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -2.4837372 | -2.8646387 | -1.1853464 |
| O     | -2.3643759 | -2.9672165 | 1.3299779  |
| O     | 0.1033073  | -2.9209341 | 2.5550547  |
| O     | 2.3451266  | -2.9556846 | 1.2442412  |
| O     | 2.2135397  | -2.9562628 | -1.5698848 |
| O     | -0.1484579 | -2.9400361 | -2.7519633 |
| O     | -3.7874041 | -0.9050962 | 2.3308782  |
| O     | 0.1826225  | -0.7783393 | 4.4157371  |
| O     | 3.8002316  | -0.7138693 | 1.9245939  |
| O     | 3.7850883  | -0.7416149 | -2.3832343 |
| O     | -0.3146462 | -0.6743270 | -4.4597421 |
| O     | -3.9461451 | -0.8497001 | -2.0755195 |
| O     | -4.4986593 | 0.7632434  | 0.0878272  |
| O     | -2.3737428 | 0.7701495  | -3.8096293 |
| O     | -2.1509698 | 0.8007715  | 3.8388637  |
| O     | 1.9566167  | 0.7827238  | -4.0264986 |
| O     | 4.4027014  | 0.6992428  | -0.1648663 |
| O     | 2.2457670  | 0.8703942  | 3.7004230  |
| O     | 1.2893887  | 2.8961599  | 2.3140383  |
| O     | 2.6063338  | 2.9056726  | -0.1834009 |
| O     | 1.2441846  | 3.0322756  | -2.4458192 |
| O     | -1.5669859 | 2.9346882  | -2.2988900 |
| O     | -2.6994923 | 2.9708768  | 0.0392194  |
| O     | -1.2267863 | 2.8587093  | 2.3525105  |
| H     | 0.2317138  | 2.8565655  | 2.2899839  |
| H     | 2.0930176  | 2.8629889  | 0.6580974  |
| H     | 1.7374186  | 2.9886773  | -1.5649198 |
| H     | -0.5819268 | 2.9527924  | -2.3288457 |
| H     | -2.2255599 | 2.9393955  | -0.8667044 |
| H     | -1.7211034 | 2.8885160  | 1.4916713  |
| H     | -2.3776831 | -2.8964524 | 0.2749090  |
| H     | -1.6398082 | -2.8687455 | -1.6947770 |
| H     | 0.7440712  | -2.9460622 | -2.2765401 |
| H     | 2.2187552  | -2.9518639 | -0.5836436 |
| H     | 1.4396911  | -2.9415620 | 1.7194040  |
| H     | -0.7638617 | -2.9087581 | 2.0700922  |
| H     | -3.8830886 | 1.5320542  | 0.0899878  |
| H     | -4.1930008 | -0.2467580 | -1.3235774 |
| H     | -4.2568269 | 0.2348498  | 0.8781865  |
| H     | -3.2259015 | 3.7846469  | 0.0250287  |
| H     | -3.4439817 | -0.2846657 | -2.7063820 |
| H     | -3.0408360 | -2.0969597 | -1.5441228 |
| H     | -3.2991039 | -1.7027430 | 1.9661851  |
| H     | -2.7353820 | -3.8421780 | 1.5231939  |
| H     | -1.5650392 | 0.2009153  | -4.0779891 |
| H     | -1.8499571 | 2.1695602  | -2.8646260 |
| H     | -2.8256024 | 0.9927115  | -4.6373130 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -0.2431775 | -1.4656403 | -3.8774162 |
| H | -0.1662644 | -3.7513727 | -3.2818973 |
| H | 0.5330926  | -0.1646185 | -4.3354068 |
| H | 1.7242969  | 1.5761405  | -3.4904919 |
| H | 2.6035138  | 0.2843113  | -3.4837359 |
| H | 2.7700441  | -2.1926929 | -1.8471346 |
| H | 4.0830945  | -0.2081900 | -1.5938849 |
| H | 4.5902497  | -1.0025184 | -2.8551138 |
| H | 1.5185019  | 3.8655418  | -2.8577221 |
| H | -2.7612885 | 0.2037225  | 3.3445060  |
| H | -1.6131991 | 2.1079542  | 2.8906708  |
| H | -4.6050311 | -1.2418825 | 2.7265409  |
| H | -1.3924532 | 0.2338371  | 4.0937092  |
| H | 0.9511205  | -0.1758077 | 4.2190331  |
| H | 3.2293702  | 2.1434630  | -0.1648190 |
| H | 4.1768150  | 0.1318016  | 0.6586874  |
| H | 5.3170322  | 0.9961715  | -0.0413176 |
| H | 3.2832632  | -1.5342859 | 1.7079451  |
| H | 2.7666762  | -3.7842792 | 1.5193923  |
| H | 0.0762885  | -2.1826400 | 3.2039749  |
| H | 0.2824471  | -1.0562110 | 5.3386688  |
| H | 1.8820359  | 1.6774913  | 3.1975616  |
| H | 1.4971561  | 3.7758785  | 2.6657973  |
| H | 3.2480258  | -0.1958214 | 2.5536890  |
| H | 2.7988798  | 1.2255338  | 4.4128943  |

### 3. Sr<sup>2+</sup> hydrate complexes with a first and second solvation shells

#### 3.1. [Sr:6/18:0/0]<sup>2+</sup> (CN=6)

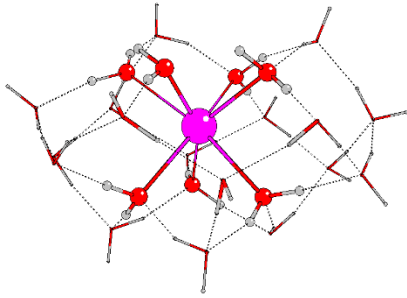


SCF Energy = -1866.2509240457

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -2.4968628 | -2.9724378 | -1.3697446 |
| O     | -3.3320624 | -3.9355399 | 0.9780746  |
| H     | -2.9533087 | -3.5198952 | 0.1450184  |
| H     | -3.7495385 | -3.1851039 | 1.4851173  |
| H     | -1.8673769 | -2.2321917 | -1.3582566 |
| H     | -3.3596172 | -2.6047573 | -1.7035856 |
| O     | -5.6793663 | -4.9714651 | -1.4548375 |
| O     | -5.0877927 | -2.4092956 | -1.9437323 |
| H     | -5.3553166 | -2.0344132 | -2.7991437 |
| H     | -5.6459805 | -1.9556534 | -1.2322990 |
| H     | -4.7469645 | -6.0219837 | -2.6515669 |
| O     | -4.0554712 | -6.6870932 | -2.8946656 |
| H     | -4.2961252 | -7.0326862 | -3.7702569 |
| O     | -1.5484648 | -5.5220323 | -2.2164946 |
| H     | -1.8157190 | -4.5945319 | -2.0199187 |

|    |            |             |            |
|----|------------|-------------|------------|
| H  | -2.3616028 | -5.9463197  | -2.5761042 |
| O  | -1.3050658 | -5.3516827  | 2.1938096  |
| H  | -1.8651260 | -4.6144016  | 1.8428570  |
| H  | -0.6851761 | -4.9520669  | 2.8264332  |
| O  | -4.2550053 | -7.9591723  | -0.5201912 |
| H  | -3.4012706 | -8.4488252  | -0.3017299 |
| H  | -4.1761265 | -7.6931305  | -1.4782807 |
| O  | -0.5021489 | -6.8909484  | -0.0633943 |
| H  | -0.8709142 | -6.3761259  | -0.8332214 |
| H  | -0.6489713 | -6.3226115  | 0.7285740  |
| O  | -1.9661214 | -9.0874751  | 0.2305256  |
| H  | -1.3308081 | -8.3076237  | 0.1175810  |
| H  | -1.6207963 | -9.8150944  | -0.3124040 |
| H  | -2.6420642 | -6.3492739  | 2.7649993  |
| O  | -3.5203731 | -6.8187616  | 2.7740589  |
| H  | -3.3059254 | -7.8169947  | 2.8245943  |
| H  | -2.6369118 | -9.5071494  | 1.9196895  |
| O  | -3.0546949 | -9.3913751  | 2.8054827  |
| H  | -3.9716185 | -9.7847743  | 2.7500284  |
| O  | -5.6538687 | -10.2217873 | 2.7651672  |
| H  | -6.0102447 | -10.0989325 | 1.8546317  |
| H  | -6.1671780 | -9.6046773  | 3.3409963  |
| O  | -5.2424909 | -6.2817132  | 4.8093553  |
| H  | -4.4315860 | -6.4997558  | 4.2765409  |
| H  | -4.9364667 | -6.0045542  | 5.6890185  |
| O  | -7.0357764 | -8.3393527  | 4.4077622  |
| H  | -6.3909352 | -7.6501059  | 4.7165759  |
| H  | -7.3750399 | -8.7612169  | 5.2150964  |
| O  | -8.9000190 | -7.0887927  | 2.7628352  |
| H  | -8.3360695 | -7.4735880  | 3.4811983  |
| H  | -9.0048934 | -6.1301800  | 2.9616225  |
| H  | -7.1142854 | -4.4642433  | 2.9011764  |
| H  | -7.9450737 | -7.1034933  | 1.4679356  |
| O  | -6.1253225 | -4.6358782  | 2.8424809  |
| H  | -5.8732166 | -5.0785640  | 3.6994377  |
| O  | -7.3078632 | -7.0723095  | 0.6740006  |
| H  | -7.1855279 | -8.0200093  | 0.3906584  |
| H  | -5.4342301 | -2.9493171  | 2.7360144  |
| O  | -4.9725711 | -2.2043113  | 2.2735995  |
| H  | -4.7019360 | -1.5749650  | 2.9629482  |
| H  | -6.0546398 | -1.6041675  | 0.8887552  |
| O  | -6.5562835 | -1.4552680  | 0.0515669  |
| H  | -7.3847114 | -1.9865159  | 0.1389628  |
| H  | -8.9562338 | -5.6653236  | -1.8843105 |
| O  | -8.3468057 | -5.3615782  | -1.1909966 |
| H  | -8.1951863 | -6.1319769  | -0.5816406 |
| H  | -8.8059027 | -3.8947655  | -0.3004106 |
| O  | -8.8519450 | -3.1266056  | 0.3298838  |
| H  | -9.6738312 | -2.6553254  | 0.1111264  |
| H  | -8.9389444 | -3.7927657  | 1.9384324  |
| O  | -8.7692530 | -4.2628070  | 2.8030629  |
| H  | -9.1471882 | -3.7026266  | 3.5011041  |
| H  | -6.6608329 | -5.0872525  | -1.5829228 |
| O  | -6.4133937 | -9.5646058  | 0.1055362  |
| H  | -5.5904921 | -9.2026465  | -0.3103566 |
| H  | -6.7925407 | -10.1953131 | -0.5288652 |
| H  | -5.4845823 | -4.0235474  | -1.7261619 |
| Sr | -5.0093616 | -5.9149505  | 0.8722704  |

### 3.2. [Sr:7/17:0/0]<sup>2+</sup> (CN=7)



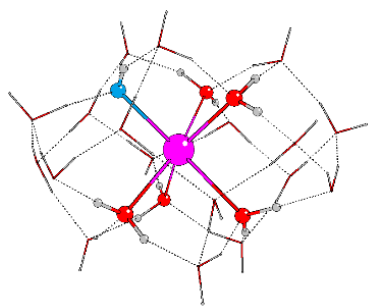
SCF Energy = -1866.2486508991

| Atoms | X          | Y           | Z          |
|-------|------------|-------------|------------|
| O     | -2.3204644 | -3.1843387  | -1.3574226 |
| O     | -3.4503533 | -4.2540948  | 0.8613335  |
| Sr    | -5.2111372 | -6.2587990  | 0.7830954  |
| O     | -3.7588109 | -6.8576141  | 2.9020221  |
| O     | -7.8200883 | -6.7682547  | 0.5178945  |
| O     | -3.8830787 | -7.9168981  | -0.6298721 |
| O     | -5.6249222 | -5.1600724  | -1.5688951 |
| O     | -6.2526554 | -4.6579912  | 2.6250704  |
| O     | -3.1190029 | -9.4161219  | 3.0962721  |
| O     | -9.2389617 | -6.7176517  | 2.7543999  |
| O     | -1.8416705 | -9.2156520  | 0.5752222  |
| O     | -0.3715640 | -6.9990011  | 0.2523728  |
| O     | -8.8458120 | -3.9145631  | 2.5084532  |
| O     | -4.8799072 | -2.6043126  | -2.0987548 |
| O     | -6.4111030 | -1.4543315  | -0.1882898 |
| O     | -3.7429523 | -6.6578752  | -3.0398292 |
| O     | -6.0290919 | -8.7818297  | 0.9223951  |
| O     | -8.3735218 | -5.1272891  | -1.5303642 |
| O     | -5.5052786 | -6.0946407  | 4.8117253  |
| O     | -4.8725678 | -2.3028183  | 2.0164928  |
| O     | -1.5116981 | -5.4326250  | 2.3268988  |
| O     | -8.7682068 | -2.8752025  | -0.0444107 |
| O     | -5.9463531 | -10.0225197 | 3.3029923  |
| O     | -1.2183252 | -5.7035141  | -2.0776042 |
| O     | -7.4216875 | -8.0194427  | 4.5367457  |
| H     | -2.9885099 | -3.8750791  | 0.0600511  |
| H     | -3.8974361 | -3.4589513  | 1.2919515  |
| H     | -1.7265962 | -2.4298912  | -1.2086662 |
| H     | -3.1509288 | -2.8136531  | -1.7568215 |
| H     | -5.0859066 | -2.2941539  | -2.9963042 |
| H     | -5.4397937 | -2.0603571  | -1.4733314 |
| H     | -4.5142683 | -6.1115232  | -2.7506292 |
| H     | -3.9708884 | -7.0158285  | -3.9132512 |
| H     | -1.4919895 | -4.7767283  | -1.8884895 |
| H     | -2.0145951 | -6.0948434  | -2.5024298 |
| H     | -2.1073186 | -4.8017866  | 1.8361163  |
| H     | -0.9893707 | -4.8992913  | 2.9485995  |
| H     | -3.1116750 | -8.4598520  | -0.3095834 |
| H     | -3.7250234 | -7.6858342  | -1.5777529 |
| H     | -0.6894140 | -6.5443259  | -0.5734001 |
| H     | -0.6491326 | -6.4115092  | 0.9949106  |
| H     | -1.1942467 | -8.4481631  | 0.4782167  |
| H     | -1.4339201 | -9.9782503  | 0.1330783  |
| H     | -2.8915453 | -6.3680378  | 2.8846741  |
| H     | -3.5065087 | -7.8318785  | 3.0164518  |
| H     | -2.7088404 | -9.5655119  | 2.2109146  |
| H     | -3.9921025 | -9.8648475  | 3.1039086  |

|   |            |             |            |
|---|------------|-------------|------------|
| H | -6.3480190 | -10.9011797 | 3.4022727  |
| H | -6.5037613 | -9.3985733  | 3.8422714  |
| H | -4.7057677 | -6.4022246  | 4.3006353  |
| H | -5.1860147 | -5.7550263  | 5.6639579  |
| H | -6.7452535 | -7.3382642  | 4.8020077  |
| H | -7.8555694 | -8.2900334  | 5.3637886  |
| H | -8.6673878 | -7.0992898  | 3.4649696  |
| H | -9.2678837 | -5.7461962  | 2.9015854  |
| H | -7.2122163 | -4.3746956  | 2.6375523  |
| H | -8.3957569 | -6.7518725  | 1.3518041  |
| H | -6.0577613 | -5.0054607  | 3.5358573  |
| H | -7.6237930 | -7.7191448  | 0.3816656  |
| H | -5.4535105 | -2.9943169  | 2.4162426  |
| H | -5.4229078 | -1.8991735  | 1.3003653  |
| H | -6.5660617 | -0.4967857  | -0.2501543 |
| H | -7.3131021 | -1.8793295  | -0.1722756 |
| H | -8.9873519 | -5.3800798  | -2.2397877 |
| H | -8.3972435 | -5.8568968  | -0.8518609 |
| H | -8.7334839 | -3.6503020  | -0.6735559 |
| H | -9.5572039 | -2.3653088  | -0.2953892 |
| H | -8.9470462 | -3.4922061  | 1.6123976  |
| H | -9.1159695 | -3.2443401  | 3.1576970  |
| H | -6.5942079 | -5.1995325  | -1.7834598 |
| H | -5.4430400 | -9.1994260  | 0.2665172  |
| H | -6.0440379 | -9.3684374  | 1.7300016  |
| H | -5.3574002 | -4.2237534  | -1.7955732 |

#### 4. Sr<sup>2+</sup> hydroxide complexes with first and second solvation shells

##### 4.1. [Sr:5/18:1/0]<sup>+</sup>

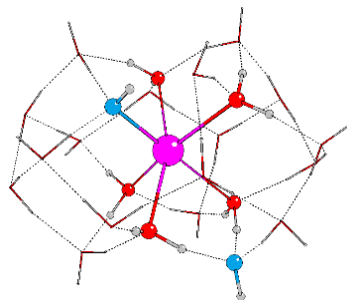


SCF Energy = -1865.7917395895

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -0.5709520 | 2.3587837  | -0.9933930 |
| O     | -0.9103928 | 3.5318123  | 1.4027714  |
| O     | 1.7294004  | 3.7735637  | 2.1303256  |
| O     | 1.3436126  | 3.6456420  | -2.2800094 |
| O     | 3.2182023  | 3.4545104  | -0.2884041 |
| O     | -2.5114052 | 1.4694983  | -2.6356595 |
| O     | -2.3482181 | -0.4617935 | -0.9667516 |
| O     | -2.7428328 | -2.6846803 | -2.1801431 |
| O     | -0.8756233 | -2.2343454 | -4.1783712 |
| O     | -1.8440261 | -4.0617440 | 0.0361705  |
| O     | 0.3555921  | -2.6262195 | -0.0724325 |
| O     | 1.4486505  | -2.7515191 | -2.5709307 |

|    |            |            |            |
|----|------------|------------|------------|
| O  | -0.9462958 | 0.4760751  | -4.7041300 |
| O  | 1.4226201  | 1.4636594  | -4.0536638 |
| O  | 1.7766762  | -0.1408435 | -1.9498382 |
| O  | 3.8515149  | 0.6965731  | -0.3788130 |
| O  | 2.0357148  | -0.1272642 | 1.4706701  |
| O  | 1.7655507  | -2.7041271 | 2.2778056  |
| O  | -0.3657672 | -2.4664874 | 3.9765017  |
| O  | -0.2999791 | 0.2102933  | 4.4552815  |
| O  | 2.1003369  | 1.4365570  | 3.6028675  |
| O  | -1.2373651 | 0.9051899  | 2.0365217  |
| O  | -3.6466134 | -0.4357041 | 1.7520811  |
| O  | -2.7328015 | -2.9867710 | 2.4058163  |
| H  | 2.0814095  | -1.7783217 | 2.0846783  |
| H  | 0.9279395  | -2.8785874 | 0.6967843  |
| H  | 1.1345765  | -2.9493389 | -1.6483312 |
| H  | 1.8381793  | -1.0794207 | -2.2819227 |
| H  | 3.2856168  | 0.3381438  | -1.1129575 |
| H  | 2.8428349  | 0.0861962  | 0.9290961  |
| H  | -0.9110211 | 3.2945739  | 0.4326066  |
| H  | -1.3478480 | 2.2473267  | -1.6140904 |
| H  | -2.5984897 | 0.6712265  | -1.9717725 |
| H  | -3.0222834 | -0.4207753 | -0.2617022 |
| H  | -2.8990215 | 0.1808600  | 1.9563095  |
| H  | -1.2614550 | 1.8981085  | 1.9697102  |
| H  | 3.5538391  | 2.5271949  | -0.2749387 |
| H  | 2.0977000  | 3.5824274  | -1.6293178 |
| H  | 2.7376437  | 3.5766608  | 0.5658846  |
| H  | 4.7466784  | 0.3459144  | -0.5181974 |
| H  | 1.5258316  | 2.9913546  | -2.9950814 |
| H  | 0.1284498  | 2.8895944  | -1.5031731 |
| H  | 0.7628356  | 3.8416596  | 1.9068371  |
| H  | -1.5635946 | 4.2408554  | 1.5224640  |
| H  | 0.5272977  | 1.1206011  | -4.3865777 |
| H  | 1.7152550  | 0.4355399  | -2.7723258 |
| H  | 2.0496060  | 1.3786096  | -4.7904684 |
| H  | -1.5839678 | 0.8482560  | -4.0410109 |
| H  | -3.3951977 | 1.8516480  | -2.7573757 |
| H  | -0.9222596 | -0.5046511 | -4.5216881 |
| H  | -0.0401405 | -2.4904799 | -3.7261073 |
| H  | -1.5888856 | -2.4445973 | -3.5177513 |
| H  | -2.6538845 | -1.7601882 | -1.7043823 |
| H  | -2.3226214 | -3.6588936 | -0.7361461 |
| H  | -3.6633973 | -2.7572882 | -2.4805540 |
| H  | 2.1530228  | -3.3902599 | -2.7693100 |
| H  | 1.9158492  | 2.3345271  | 3.2268931  |
| H  | 2.0944368  | 0.4683206  | 2.2894873  |
| H  | 1.9557882  | 4.6088527  | 2.5727976  |
| H  | 1.2860454  | 1.1524831  | 4.0783227  |
| H  | -0.3175818 | -0.7882408 | 4.4313295  |
| H  | -0.4657115 | -3.2288943 | -0.0218498 |
| H  | -2.2624404 | -3.6875509 | 0.8603966  |
| H  | -3.1092139 | -2.0848071 | 2.2428514  |
| H  | -4.4243866 | -0.0679274 | 2.2028463  |
| H  | -0.9397611 | 0.6991989  | 2.9713972  |
| H  | -0.8222669 | 0.4786037  | 5.2290460  |
| H  | 0.4592900  | -2.6606468 | 3.4529215  |
| H  | 2.5522544  | -3.2306122 | 2.4963759  |
| H  | -1.9396312 | -2.8401843 | 2.9717640  |
| H  | -0.3249149 | -3.0393679 | 4.7606680  |
| Sr | -0.0949931 | -0.0548649 | -0.1117613 |

## 4.2 [Sr:5/17:1/1]

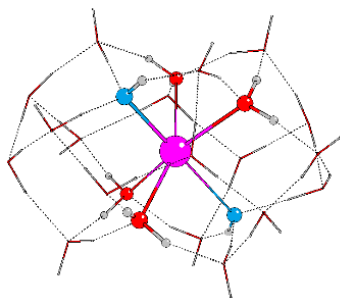


SCF Energy = -1865.3280926845

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -0.5600265 | 2.3520287  | -1.0265978 |
| Sr    | -0.9203225 | 3.4809091  | 1.3182027  |
| O     | 1.5411528  | 3.3866810  | 1.3432326  |
| O     | 1.9805798  | 3.2406466  | -1.1623884 |
| O     | 2.7449073  | 5.4294764  | 2.3097708  |
| O     | -0.8767983 | 5.2476394  | 3.2128611  |
| O     | -0.8398151 | 0.9908504  | 2.1309096  |
| O     | -1.8899694 | 5.5161908  | -0.0469807 |
| O     | 1.3703659  | 5.2133859  | 4.7115913  |
| O     | -2.0753219 | 3.1685079  | -3.0401394 |
| O     | -3.3907693 | 3.4069638  | 2.1872948  |
| O     | -4.5806999 | 0.9418269  | 2.2909275  |
| O     | -1.0433509 | 5.7616931  | -2.5732304 |
| O     | 1.5215595  | 5.8713123  | -1.9075055 |
| O     | -2.4779602 | 0.2632539  | 4.1258871  |
| O     | -1.3104331 | -0.1349936 | -0.3019849 |
| O     | -0.9131994 | 7.3971118  | 1.6270629  |
| O     | -2.8500966 | 4.2851836  | 4.5035209  |
| O     | -4.5344522 | 4.8305560  | 0.0989751  |
| O     | -1.8075903 | 2.3061857  | 5.7177959  |
| O     | -4.4625924 | 2.7272996  | -1.7939032 |
| O     | -4.1154572 | 0.3738287  | -0.3718150 |
| O     | 0.9909623  | 2.6015347  | 5.5184154  |
| O     | 1.7019220  | 7.2366646  | 0.4894612  |
| O     | 1.6674342  | 1.0587156  | 3.2752985  |
| H     | -3.3268732 | 3.8075143  | 3.1536199  |
| H     | -1.6813784 | 4.9830325  | 3.8224544  |
| H     | -0.9432231 | 6.7310223  | 2.3777379  |
| H     | -1.6526209 | 6.3442654  | 0.4563166  |
| H     | -3.6557968 | 5.2763224  | -0.0327633 |
| H     | -3.9743973 | 3.9865573  | 1.6422010  |
| H     | -0.9218207 | 0.6686853  | -0.7472685 |
| H     | 0.3962530  | 2.5407829  | -1.2493490 |
| H     | 1.9413860  | 3.2543513  | -0.1166755 |
| H     | 1.8679570  | 2.6199357  | 1.8508905  |
| H     | 0.7993881  | 0.8496599  | 2.8430161  |
| H     | -0.9686535 | 0.3962170  | 1.3427805  |
| H     | -4.5979928 | 3.4522481  | -1.1387666 |
| H     | -2.9858346 | 3.0818268  | -2.6344979 |
| H     | -4.3455883 | 1.8956885  | -1.2567366 |
| H     | -5.2047305 | 5.5331925  | 0.0871509  |
| H     | -1.8455382 | 4.1265778  | -3.0309467 |
| H     | -1.1055891 | 2.6341001  | -1.8326272 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -3.1716657 | 0.0969826  | -0.4214047 |
| H | -0.8547902 | -0.9091130 | -0.6712777 |
| H | -0.0468319 | 5.8399318  | -2.4017518 |
| H | -1.6206155 | 5.6825242  | -1.0001560 |
| H | -1.3079475 | 6.5571913  | -3.0633874 |
| H | 1.7801567  | 4.9380059  | -1.6882806 |
| H | 2.7631666  | 2.7294603  | -1.4231490 |
| H | 1.5856392  | 6.3693927  | -1.0452347 |
| H | 0.8128070  | 7.4136269  | 0.8749050  |
| H | 2.1415147  | 6.6353698  | 1.1494240  |
| H | 2.3144598  | 4.5682302  | 1.9026215  |
| H | 2.0036197  | 5.2575088  | 3.9492843  |
| H | 3.7071524  | 5.3073194  | 2.2649525  |
| H | -1.3712825 | 8.1953645  | 1.9363800  |
| H | -4.2126414 | 1.8677209  | 2.2698709  |
| H | -4.2851465 | 0.5095496  | 0.6003623  |
| H | -3.9942947 | 0.4950430  | 2.9402488  |
| H | -2.2764831 | 0.9663815  | 4.8195798  |
| H | -0.0644959 | 5.2714144  | 3.8040348  |
| H | 1.3324391  | 4.2592391  | 4.9961384  |
| H | 1.2489306  | 1.9982917  | 4.7777516  |
| H | 2.1149268  | 0.2052949  | 3.3963743  |
| H | -1.4475430 | 0.6444854  | 2.8511846  |
| H | -2.2929407 | -0.5956078 | 4.5394205  |
| H | -2.2828473 | 3.1468750  | 5.3018739  |
| H | -3.4661168 | 4.8583456  | 4.9845252  |
| H | 0.0102816  | 2.4933207  | 5.6159441  |
| H | -2.1024111 | 2.2464775  | 6.6410816  |

### 4.3 [Sr:4/18:2/0]



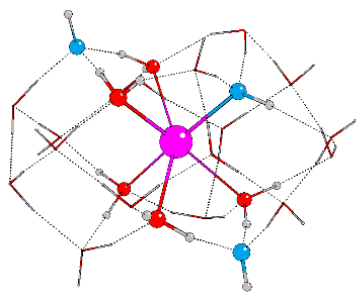
SCF Energy = -1865.3269565274

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| Sr    | -0.6346070 | 2.2865056  | -1.0334767 |
| O     | -1.0292426 | 3.4467859  | 1.3151426  |
| H     | -0.2507289 | 3.7076580  | 1.8890594  |
| H     | -1.5477985 | 4.2811512  | 1.1535978  |
| H     | -2.7887919 | 1.6114854  | 3.4030318  |
| H     | -1.9013554 | 2.2363220  | 2.2701771  |
| O     | -2.2563674 | 1.3786989  | 2.6250259  |
| O     | -2.5552626 | 0.8450739  | -0.3294807 |
| H     | -2.7249446 | 0.9254590  | 0.6283105  |
| H     | 1.2255758  | -0.9468731 | -4.0820143 |
| H     | 0.7890419  | -0.4640500 | -2.6404536 |
| O     | -2.4177655 | -1.6566105 | -0.7914273 |
| H     | -2.5311686 | -0.6325264 | -0.5780670 |



|   |            |            |            |
|---|------------|------------|------------|
| H | -3.2211333 | -2.0982208 | -0.4712971 |
| O | -2.2307521 | -1.4221249 | -3.5429910 |
| H | -1.2773643 | -1.2016780 | -3.6522349 |
| H | -2.3354450 | -1.5750737 | -2.5648817 |
| O | -4.3953064 | 1.8542202  | -1.7580414 |
| H | -3.7336774 | 1.3795256  | -1.0911396 |
| H | -5.2770714 | 1.8528670  | -1.3527873 |
| O | -2.6246400 | 3.8799487  | -1.7180001 |
| H | -2.6063618 | 4.3814108  | -2.5972670 |
| H | -3.4264603 | 3.2822854  | -1.7469679 |
| O | -2.2542120 | 2.6009821  | -5.2572825 |
| H | -2.1223181 | 2.4518806  | -6.2077423 |
| H | -2.9027627 | 1.8904706  | -4.9362062 |
| O | -3.8266492 | 0.7315661  | -4.2212165 |
| H | -4.1274072 | 1.1013771  | -3.3493062 |
| H | -3.2496650 | -0.0475953 | -3.9853231 |
| O | -2.4258217 | 5.1502793  | -4.0387868 |
| H | -1.5100911 | 5.5431194  | -3.9379246 |
| H | -2.3395525 | 4.3687429  | -4.6324745 |
| O | 0.0170194  | 6.2330861  | -3.5095292 |
| H | 0.0159045  | 6.4449436  | -2.5349870 |
| H | 0.6869072  | 5.5150631  | -3.6296485 |
| O | 1.7345222  | 4.0427262  | -3.8365047 |
| H | 2.3013834  | 4.0084626  | -4.6242393 |
| H | 1.1027178  | 3.2818027  | -3.9218562 |
| O | 1.6565165  | 3.2577171  | -0.9453434 |
| H | 1.9800838  | 3.4835539  | -1.8379622 |
| O | 1.9433553  | 5.4907218  | 0.4117971  |
| H | 1.7470657  | 5.2060698  | 1.3282451  |
| H | 1.8562064  | 4.6232116  | -0.1227092 |
| O | -0.0444706 | 6.8922953  | -0.8198336 |
| H | 0.6745597  | 6.4036566  | -0.3225855 |
| H | -0.8831460 | 6.5742692  | -0.4155293 |
| O | 2.9355201  | 1.3902032  | 0.1093496  |
| H | 2.4962875  | 2.2519487  | -0.3725811 |
| H | 3.8726772  | 1.3460938  | -0.1379628 |
| O | 0.8393129  | 0.0908332  | -0.9872696 |
| H | 1.7329501  | 0.3861034  | -0.6542156 |
| H | 0.5490412  | -0.6680105 | -0.3826993 |
| O | -0.0517345 | -1.8355843 | 0.6142838  |
| H | -0.1268552 | -1.3279328 | 1.4687198  |
| H | -0.9672127 | -1.8828101 | 0.2300733  |
| O | -0.0489731 | -0.3024923 | 2.9058612  |
| H | -0.8338814 | 0.3018678  | 2.8831528  |
| H | 0.7382677  | 0.2906778  | 2.8468264  |
| O | 2.1760398  | 1.4742917  | 2.6585384  |
| H | 2.5748815  | 1.4150111  | 1.7328519  |
| H | 2.8949409  | 1.2628417  | 3.2769154  |
| O | 1.1630236  | 3.9933432  | 2.7870445  |
| H | 1.0053156  | 4.2877014  | 3.6989168  |
| H | 1.6068344  | 3.0999986  | 2.8511748  |
| O | -2.3426530 | 5.6119096  | 0.3178101  |
| H | -3.1257307 | 6.0367712  | 0.7041368  |
| H | -2.6616738 | 5.0614517  | -0.4518065 |
| O | 0.4930294  | -0.5401305 | -3.5912096 |
| O | -0.1902769 | 2.0818356  | -3.6232411 |
| H | 0.1294912  | 1.1553148  | -3.8017342 |
| H | -0.9112475 | 2.2585814  | -4.2982290 |

#### 4.4 [Sr:5/16:1/2]

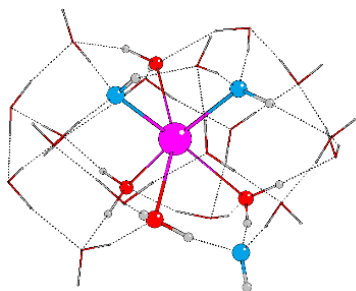


SCF Energy = -1864.8602673114

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -0.4680023 | 2.4388458  | -1.0220830 |
| Sr    | -0.8898481 | 3.2647979  | 1.4015730  |
| O     | 1.5436736  | 3.5454639  | 1.5901776  |
| O     | -0.7684224 | 5.5341894  | 0.1045374  |
| O     | -1.2258188 | 4.5952174  | -2.1745880 |
| O     | -2.4907902 | 7.4517437  | 0.7161633  |
| O     | 1.7255426  | 6.0291275  | 1.1673658  |
| O     | 2.1438093  | 1.8099036  | -0.2726875 |
| O     | -2.2004390 | 4.6062375  | 3.2250759  |
| O     | -1.1168134 | 3.4393370  | 5.2029275  |
| O     | 1.1311668  | 4.6376576  | 5.3582563  |
| O     | -0.7870510 | 1.6230113  | 3.4262557  |
| O     | 1.5832987  | -0.4304808 | 1.0374277  |
| O     | -4.6717987 | 4.1891613  | 2.3209367  |
| O     | -3.3129948 | 2.1988261  | 1.0539374  |
| O     | -1.8142695 | 0.2045918  | -1.8528128 |
| O     | 2.7771172  | 2.8391497  | 4.1844290  |
| O     | -4.1113779 | 1.8139869  | -1.4912438 |
| O     | -3.8397890 | 4.3388824  | -2.1847742 |
| O     | -1.6998456 | 7.2735324  | 3.4063295  |
| O     | -2.6467002 | -0.1405944 | 2.4515088  |
| O     | 1.6077630  | 0.3550967  | 3.7216905  |
| O     | -1.0875496 | -1.2004826 | 0.4098823  |
| O     | 1.0079071  | 6.9136681  | 3.6913209  |
| O     | -4.7162195 | 5.8676352  | 0.0265861  |
| H     | -0.9291216 | 2.2474501  | 4.2421690  |
| H     | -1.8538336 | 4.1787511  | 4.1177104  |
| H     | -3.8253138 | 4.4014977  | 2.8217992  |
| H     | -3.9752399 | 2.7870275  | 1.5041851  |
| H     | -3.0963105 | 0.5706094  | 1.9341601  |
| H     | -1.9842251 | 0.3897119  | 2.9700260  |
| H     | 1.3129500  | 1.9661332  | -0.7855085 |
| H     | -0.7268637 | 3.2505168  | -1.6149397 |
| H     | -0.8824371 | 5.2441208  | -0.9165791 |
| H     | 0.1588756  | 5.8480935  | 0.2630012  |
| H     | 1.7634815  | 4.9823926  | 1.3339654  |
| H     | 2.0307013  | 2.5001197  | 0.4793796  |
| H     | -1.6289837 | -0.8704961 | 1.1769596  |
| H     | -1.6427779 | -0.3368339 | -1.0338219 |
| H     | -0.1543030 | -0.9483109 | 0.6183623  |
| H     | -2.7098203 | 0.6026180  | -1.7513734 |
| H     | -0.9379973 | 1.6403309  | -1.3909316 |
| H     | 1.8485204  | 0.3861838  | 0.4947948  |
| H     | -4.0516086 | 2.7797614  | -1.8167636 |
| H     | -3.6738219 | 2.0287664  | 0.1358448  |
| H     | -5.0290136 | 1.5277139  | -1.6274389 |
| H     | -2.8290255 | 4.4802518  | -2.2339748 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -0.7576068 | 4.9548803  | -2.9432305 |
| H | -4.1441044 | 4.8757910  | -1.4087533 |
| H | -4.7997110 | 5.3060156  | 0.8327950  |
| H | -3.9890263 | 6.5015080  | 0.2468614  |
| H | -1.7965388 | 6.7810262  | 0.4148698  |
| H | -1.9176005 | 7.5172888  | 2.4742054  |
| H | -2.3437619 | 8.2529142  | 0.1872221  |
| H | -5.3765092 | 4.0960788  | 2.9821081  |
| H | 1.7375858  | 0.0773575  | 2.7796139  |
| H | 0.0767316  | 1.1435449  | 3.5799197  |
| H | 2.2156255  | -1.1283663 | 0.7989949  |
| H | 2.1591378  | 1.1637676  | 3.8589925  |
| H | 2.2352804  | 3.5065947  | 4.6997307  |
| H | -2.0388562 | 5.5914197  | 3.3133106  |
| H | -0.7040540 | 7.2255095  | 3.4628024  |
| H | 1.3421949  | 6.6232819  | 2.8012137  |
| H | 2.5551688  | 6.2864154  | 0.7349639  |
| H | 2.0017829  | 3.3207540  | 2.4251857  |
| H | 3.7087843  | 3.0512693  | 4.3523939  |
| H | 0.1983602  | 4.1583934  | 5.3839341  |
| H | -1.6214232 | 3.2747070  | 6.0139087  |
| H | 1.0684273  | 6.1129330  | 4.2730984  |
| H | 1.3447053  | 4.8750832  | 6.2751863  |

#### 4.5. [Sr:4/17:2/1]

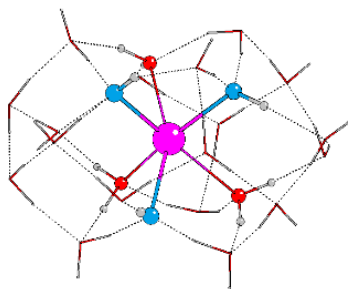


SCF Energy = -1864.8613269723

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -0.4887090 | 2.3940342  | -1.0716936 |
| Sr    | -0.8973291 | 3.3607683  | 1.3566103  |
| O     | 1.5463312  | 3.5429430  | 1.5475620  |
| O     | -0.8206066 | 5.5022090  | 0.0656184  |
| O     | -2.4806506 | 7.3210998  | 0.6700544  |
| O     | -1.2948277 | 4.6850473  | -2.2834330 |
| O     | 1.8532144  | 6.0562824  | 1.2209300  |
| O     | 2.1510721  | 1.7899674  | -0.2720671 |
| O     | 1.5763932  | -0.4450806 | 1.0357375  |
| O     | -2.2383125 | 4.6147746  | 3.2437460  |
| O     | -1.7141631 | 7.2814790  | 3.3326172  |
| O     | -1.8294953 | 0.1811529  | -1.8119370 |
| O     | -0.7792298 | 1.6698359  | 3.3946627  |
| O     | 1.6031080  | 0.3618895  | 3.7114500  |
| O     | -1.1180907 | 3.4554954  | 5.2102127  |
| O     | -4.6936825 | 4.1747096  | 2.3318554  |
| O     | -3.3105720 | 2.2178473  | 1.0390143  |
| O     | -4.1713589 | 1.7611922  | -1.4865489 |
| O     | -4.0254341 | 4.3295644  | -2.1672619 |

|   |            |            |            |
|---|------------|------------|------------|
| O | -2.6327475 | -0.1008730 | 2.4605659  |
| O | 0.9917645  | 6.9094824  | 3.6846892  |
| O | 1.1348580  | 4.6339902  | 5.3547974  |
| O | -1.0984654 | -1.2115520 | 0.4373285  |
| O | 2.7735053  | 2.8395240  | 4.1649878  |
| O | -4.7348103 | 5.8499702  | 0.0373691  |
| H | -0.9245720 | 2.2790538  | 4.2175781  |
| H | -1.8767590 | 4.1914562  | 4.1292070  |
| H | -3.8482150 | 4.3931724  | 2.8344413  |
| H | -3.9754483 | 2.7964876  | 1.4978958  |
| H | -3.0837138 | 0.5997421  | 1.9300581  |
| H | -1.9624451 | 0.4442606  | 2.9568075  |
| H | 1.3422070  | 1.9295901  | -0.8163982 |
| H | -0.7083514 | 3.1381727  | -1.6958651 |
| H | -1.0424411 | 5.1312182  | -1.3607330 |
| H | 0.0784246  | 5.8581070  | 0.2150575  |
| H | 1.8172061  | 5.0143932  | 1.3381965  |
| H | 2.0114259  | 2.4957375  | 0.4707834  |
| H | -1.6328515 | -0.8608881 | 1.2014809  |
| H | -1.6548885 | -0.3641681 | -0.9935197 |
| H | -0.1624071 | -0.9589828 | 0.6336617  |
| H | -2.7360513 | 0.5542557  | -1.7226890 |
| H | -0.9685623 | 1.5805349  | -1.4123089 |
| H | 1.8434181  | 0.3731542  | 0.4953495  |
| H | -4.1651329 | 2.7207240  | -1.8114049 |
| H | -3.6905850 | 2.0241365  | 0.1359782  |
| H | -5.0820433 | 1.4395076  | -1.5863692 |
| H | -3.0540732 | 4.5093729  | -2.2849240 |
| H | -0.8416774 | 5.1784236  | -2.9852461 |
| H | -4.2899891 | 4.8664513  | -1.3692045 |
| H | -4.8259123 | 5.2867370  | 0.8415253  |
| H | -3.9580969 | 6.4395668  | 0.2407196  |
| H | -1.7617687 | 6.6008895  | 0.3807353  |
| H | -1.9235887 | 7.4474395  | 2.3766744  |
| H | -2.3300054 | 8.1033271  | 0.1150616  |
| H | -5.3963371 | 4.0634569  | 2.9922678  |
| H | 1.7301899  | 0.0769049  | 2.7712580  |
| H | 0.0801405  | 1.1855035  | 3.5479343  |
| H | 2.2097896  | -1.1422344 | 0.7983407  |
| H | 2.1585628  | 1.1686941  | 3.8431773  |
| H | 2.2320100  | 3.5084834  | 4.6791144  |
| H | -2.0698884 | 5.6002414  | 3.3159625  |
| H | -0.7207816 | 7.2168118  | 3.4018425  |
| H | 1.3631887  | 6.6171482  | 2.8066845  |
| H | 2.7529518  | 6.2740370  | 0.9299713  |
| H | 1.9830645  | 3.3036847  | 2.3894724  |
| H | 3.7052162  | 3.0639374  | 4.3150461  |
| H | 0.1973928  | 4.1588534  | 5.3841766  |
| H | -1.6084332 | 3.2711744  | 6.0257112  |
| H | 1.0497676  | 6.1136930  | 4.2726073  |
| H | 1.3564058  | 4.8656667  | 6.2712711  |

#### 4.6. [Sr:3/18:3/0]

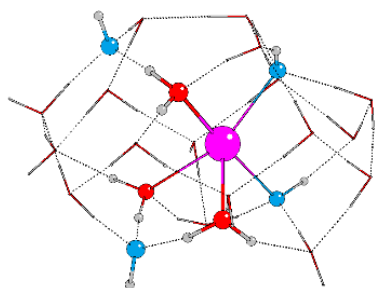


SCF Energy = -1864.8593862609

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | 1.7301519  | 0.8769268  | 1.8606126  |
| Sr    | 0.0659548  | -0.0328840 | -0.0311429 |
| O     | 1.6271077  | 0.9594245  | -1.6669815 |
| O     | 1.6920027  | -1.9388986 | 0.1372275  |
| O     | 2.6870257  | -1.5972475 | 2.4305702  |
| O     | 0.6824593  | -4.2660361 | 0.0403324  |
| O     | 2.8440484  | -1.1281487 | -2.4789489 |
| O     | 2.7675985  | 2.6476392  | -0.0568290 |
| O     | -1.7191033 | -1.5314098 | -0.9998930 |
| O     | -2.7353796 | -0.0149956 | -2.6991196 |
| O     | -0.8940136 | 0.0342595  | -4.6282432 |
| O     | -1.7181746 | 1.7874685  | -0.9560285 |
| O     | 0.8810858  | 4.4978152  | 0.1120447  |
| O     | -2.8259126 | -2.2859167 | 1.1573394  |
| O     | -1.6624965 | -0.0298173 | 2.0360938  |
| O     | 0.7200506  | 2.2004507  | 3.9842545  |
| O     | 0.4766579  | 2.3423225  | -4.0533252 |
| O     | -0.6483076 | -0.2233629 | 4.5501335  |
| O     | 0.6358604  | -2.4969629 | 4.0376150  |
| O     | -0.5963244 | -3.8289098 | -2.3983885 |
| O     | -2.8140765 | 2.4349954  | 1.4827762  |
| O     | -0.6905163 | 3.9855210  | -2.1306664 |
| O     | -0.7021212 | 3.9607576  | 2.4245260  |
| O     | 0.8792799  | -2.1639393 | -4.0822360 |
| O     | -0.9065962 | -3.9753463 | 2.2862332  |
| H     | -2.2411036 | 1.2758127  | -1.6328881 |
| H     | -2.3763481 | -0.7453511 | -1.9828089 |
| H     | -2.4566660 | -2.0307598 | 0.2033539  |
| H     | -2.2373676 | -0.8274395 | 1.8573680  |
| H     | -2.5394455 | 1.5553831  | 1.8460222  |
| H     | -2.5715163 | 2.3234978  | 0.5270870  |
| H     | 2.6225679  | 2.1169239  | 0.7613680  |
| H     | 2.2228767  | 0.0750396  | 2.1852301  |
| H     | 2.3773750  | -1.8110021 | 1.4402427  |
| H     | 2.2985648  | -1.8297258 | -0.6220159 |
| H     | 2.4073671  | -0.2199438 | -2.1810320 |
| H     | 2.3678470  | 2.0165478  | -0.7724552 |
| H     | -1.4884482 | 3.4627701  | 2.0693704  |
| H     | 0.1330927  | 2.8338642  | 3.4830976  |
| H     | -0.1422049 | 4.1613550  | 1.6343807  |
| H     | 0.1460174  | 1.4700475  | 4.3104368  |
| H     | 1.4081724  | 1.3631101  | 2.6763620  |
| H     | 1.6529872  | 3.8369065  | 0.0620340  |
| H     | -0.1532427 | -1.0997652 | 4.4354022  |
| H     | -1.3573604 | -0.1099571 | 2.9818744  |
| H     | -1.2862653 | -0.3564778 | 5.2698228  |
| H     | 1.4292381  | -2.2294035 | 3.5002003  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 3.6116349  | -1.8768226 | 2.5203558  |
| H | 0.0662378  | -3.0248675 | 3.4095350  |
| H | -1.6518705 | -3.4320658 | 1.9250661  |
| H | -0.3270449 | -4.1483441 | 1.4953021  |
| H | 1.1525494  | -3.3206563 | 0.0735935  |
| H | -0.0624029 | -4.0574269 | -1.5959055 |
| H | 1.3888609  | -4.9285537 | 0.1077315  |
| H | -3.7782482 | -2.4517249 | 1.0751965  |
| H | -0.0421243 | 4.2326519  | -1.4219262 |
| H | -1.3763663 | 2.6087352  | -1.4208883 |
| H | 1.2853745  | 5.3801209  | 0.1535679  |
| H | -0.1780456 | 3.5359079  | -2.8451828 |
| H | -0.0331196 | 1.5436163  | -4.3605871 |
| H | -1.3756030 | -2.3243189 | -1.4717456 |
| H | -0.0118687 | -3.2666513 | -2.9717531 |
| H | 1.6242868  | -1.7755352 | -3.5435956 |
| H | 3.6992660  | -0.9078348 | -2.8811009 |
| H | 1.2826370  | 1.4298542  | -2.4512352 |
| H | 1.0794954  | 2.5762396  | -4.7766415 |
| H | -1.6644766 | -0.0064198 | -3.9785201 |
| H | -3.6717662 | -0.1951040 | -2.8779749 |
| H | 0.2769782  | -1.4074127 | -4.2751973 |
| H | -1.2879321 | -0.0237052 | -5.5142724 |

#### 4.7. [Sr:3/17:2/2]<sup>2-</sup>

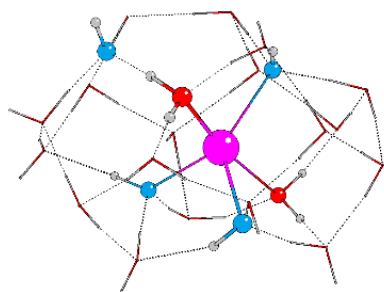


SCF Energy = -1864.3776225447

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -1.9447171 | -2.9960714 | -1.3692076 |
| O     | -1.4053434 | -1.6676655 | 1.0128454  |
| Sr    | 0.2261680  | -0.0938727 | -0.2443895 |
| O     | 0.5425264  | 1.8298897  | -1.6874437 |
| O     | 2.0024980  | -1.6019211 | 0.8904612  |
| O     | 0.7158039  | 1.6592461  | 1.6165369  |
| O     | -1.6128859 | 2.4258186  | 2.2652351  |
| O     | 2.6317150  | -2.6179704 | -1.5702948 |
| O     | 3.9607665  | -0.3192780 | 2.1340901  |
| O     | 0.4015629  | -2.6187223 | 2.5334225  |
| O     | 2.4518773  | 3.1952575  | 0.2641122  |
| O     | 1.9408721  | 1.1080391  | -3.7839613 |
| O     | -1.8730726 | 2.6387718  | -2.3052240 |
| O     | -3.8174195 | -1.2906529 | -2.1626403 |
| O     | -2.1970638 | 0.6255425  | 3.9413537  |
| O     | -2.5347877 | 0.5481222  | -3.9050859 |
| O     | 0.2833437  | -1.8048049 | -2.0356969 |
| O     | -0.0720963 | -0.5533890 | -4.6867764 |
| O     | -3.6737157 | -0.9401119 | 2.4096919  |
| O     | 0.1213502  | -0.9275213 | 4.5585577  |

|   |            |            |            |
|---|------------|------------|------------|
| O | 4.4231736  | 1.2585333  | -0.1575874 |
| O | -4.7160805 | 0.1768330  | 0.0656110  |
| O | -3.1958886 | 2.5259088  | 0.1133816  |
| O | 3.9855997  | -0.3247612 | -2.4242301 |
| O | 2.0623152  | 0.8570143  | 3.8715047  |
| H | -1.0689948 | -2.5955607 | -1.7305372 |
| H | -1.8883204 | -2.7165408 | -0.4212740 |
| H | -3.1320660 | -1.9921665 | -1.8987114 |
| H | -4.5471589 | -1.7740820 | -2.5836681 |
| H | -4.3998820 | -0.3857348 | -0.6852269 |
| H | -4.4201921 | -0.2777036 | 0.8904695  |
| H | -2.2260931 | -1.4580416 | 1.5270896  |
| H | -2.3548964 | 2.6080956  | -1.4340949 |
| H | -0.9123619 | 2.3776221  | -2.0715696 |
| H | -2.3305856 | 1.3214035  | -3.2990083 |
| H | -2.9895141 | -0.1118189 | -3.3283711 |
| H | -0.9220241 | -0.1255292 | -4.4041300 |
| H | 0.6547478  | 0.0692328  | -4.4074417 |
| H | 0.1974640  | -1.4523977 | -2.9484386 |
| H | 1.0453701  | 2.5419852  | -1.2545304 |
| H | 2.8143858  | -3.5163536 | -1.8874673 |
| H | 2.3126915  | -2.1971008 | 0.1604046  |
| H | 2.7225265  | 3.9872235  | 0.7560674  |
| H | 1.7838879  | 2.7207789  | 0.8463666  |
| H | 3.7551923  | 1.9800315  | -0.0271566 |
| H | 4.3648694  | 0.7165083  | 0.6668652  |
| H | 3.5731005  | -1.1759747 | -2.1293298 |
| H | 4.1142810  | 0.2136701  | -1.5999315 |
| H | 2.6654610  | 0.5710353  | -3.3765543 |
| H | 1.4043797  | 1.4290158  | -2.9721694 |
| H | 3.2785510  | -0.9054063 | 1.6761782  |
| H | 4.6603187  | -0.9129125 | 2.4523118  |
| H | 1.4116668  | 0.1540954  | 4.1658952  |
| H | 2.7946019  | 0.3819044  | 3.4116677  |
| H | -0.2250416 | 2.0456631  | 1.9097542  |
| H | 1.1836238  | 1.3923111  | 2.4575679  |
| H | 1.4057219  | -2.1533068 | 1.5857095  |
| H | -1.6031756 | 3.3072878  | 2.6714948  |
| H | 0.4036310  | -3.5775630 | 2.6769441  |
| H | -0.7487774 | -2.1464828 | 1.6740673  |
| H | -1.9639092 | 1.4312861  | 3.2804144  |
| H | -2.6211716 | 1.0167893  | 4.7220470  |
| H | -0.6923379 | -0.4071156 | 4.3474140  |
| H | 0.2032876  | -1.6213326 | 3.8229380  |
| H | -3.2076399 | -0.3416842 | 3.0798019  |
| H | -4.1219237 | -1.6362163 | 2.9161523  |
| H | 1.6430924  | -2.3658688 | -1.8571087 |
| H | -2.6008036 | 2.4824797  | 0.9327438  |
| H | -3.7300168 | 1.6915092  | 0.1138965  |

#### 4.8. [Sr:2/18:3/1]<sup>2-</sup>



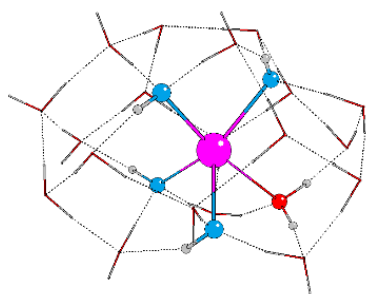
SCF Energy = -1864.3817770345

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -2.0987037 | -2.9929811 | -1.1737162 |
| O     | -1.3899699 | -1.6018519 | 0.8900547  |
| Sr    | 0.3228060  | -0.1800850 | -0.1130726 |
| O     | 0.5501259  | 1.7275779  | -1.6518550 |
| O     | 2.1656036  | -1.6332091 | 0.6895597  |
| O     | 0.7258683  | 1.6803352  | 1.6437918  |
| O     | -1.5995654 | 2.4546246  | 2.2870490  |
| O     | 2.9378204  | -2.5355497 | -1.5644984 |
| O     | 3.9045525  | -0.3366998 | 2.0074993  |
| O     | 0.1223899  | -2.8282407 | 2.5600883  |
| O     | 2.4123299  | 3.2317674  | 0.2600020  |
| O     | 1.8956598  | 1.1066405  | -3.7881264 |
| O     | -1.8482484 | 2.5729115  | -2.2555169 |
| O     | -3.8847571 | -1.2774119 | -2.1163922 |
| O     | -2.1797982 | 0.6536296  | 3.9599667  |
| O     | -2.4955876 | 0.4820139  | -3.8423759 |
| O     | 0.3352832  | -1.9043758 | -2.1467555 |
| O     | -0.0571466 | -0.6574221 | -4.4917073 |
| O     | -3.8080301 | -0.8348011 | 2.4498231  |
| O     | 0.0562218  | -0.9311742 | 4.5501808  |
| O     | 4.4470639  | 1.3492427  | -0.1450195 |
| O     | -4.7819797 | 0.2418979  | 0.0862919  |
| O     | -3.2179732 | 2.5707157  | 0.1498007  |
| O     | 4.0913307  | -0.1492586 | -2.4785787 |
| O     | 2.1059929  | 0.7555513  | 3.8291404  |
| H     | -1.2771252 | -2.8449641 | -1.6945533 |
| H     | -1.8690540 | -2.4893083 | -0.2967721 |
| H     | -3.2270734 | -1.9820712 | -1.7944144 |
| H     | -4.6094128 | -1.7623911 | -2.5441585 |
| H     | -4.4584732 | -0.3228738 | -0.6589825 |
| H     | -4.4809909 | -0.2059235 | 0.9144211  |
| H     | -2.1912906 | -1.3331233 | 1.3810509  |
| H     | -2.3396564 | 2.5680210  | -1.3895329 |
| H     | -0.8944630 | 2.2837500  | -2.0131664 |
| H     | -2.2992042 | 1.2612853  | -3.2378923 |
| H     | -2.9895521 | -0.1580378 | -3.2739013 |
| H     | -0.9220264 | -0.2058143 | -4.2815415 |
| H     | 0.6606350  | 0.0214042  | -4.3200440 |
| H     | 0.2159348  | -1.5029885 | -3.0625799 |
| H     | 1.0426945  | 2.4483537  | -1.2211596 |
| H     | 3.3928833  | -3.3919149 | -1.5371190 |
| H     | 2.6886454  | -2.2783521 | -0.5824991 |
| H     | 2.6511054  | 4.0472345  | 0.7295025  |
| H     | 1.7649814  | 2.7454621  | 0.8569894  |
| H     | 3.7601047  | 2.0527612  | -0.0214360 |
| H     | 4.3315143  | 0.7516096  | 0.6398344  |
| H     | 3.7593269  | -1.0311308 | -2.1760272 |



|   |            |            |            |
|---|------------|------------|------------|
| H | 4.1949088  | 0.3849114  | -1.6464087 |
| H | 2.6770459  | 0.6301522  | -3.4118837 |
| H | 1.3736488  | 1.3945897  | -2.9461085 |
| H | 3.2180489  | -0.9383469 | 1.4809864  |
| H | 4.6241149  | -0.9210195 | 2.2958588  |
| H | 1.4348366  | 0.0737019  | 4.1122352  |
| H | 2.7903262  | 0.2792041  | 3.2917097  |
| H | -0.2188115 | 2.0632528  | 1.9338604  |
| H | 1.1951158  | 1.3980506  | 2.4786037  |
| H | 1.7208480  | -2.2632721 | 1.2904427  |
| H | -1.5838849 | 3.3330697  | 2.6997426  |
| H | -0.2276195 | -3.7097617 | 2.7657113  |
| H | -0.5506602 | -2.3927997 | 1.8877651  |
| H | -1.9463047 | 1.4574710  | 3.2942787  |
| H | -2.5863073 | 1.0523877  | 4.7462465  |
| H | -0.7385566 | -0.3728464 | 4.3443818  |
| H | 0.0480957  | -1.6580802 | 3.8682525  |
| H | -3.2585744 | -0.2886790 | 3.0916593  |
| H | -4.1582031 | -1.5868938 | 2.9520923  |
| H | 1.2449754  | -2.2995889 | -2.1182528 |
| H | -2.6087880 | 2.5105524  | 0.9560980  |
| H | -3.7538469 | 1.7374025  | 0.1454934  |

#### 4.9. [Sr:1/19:4/0]<sup>2-</sup>

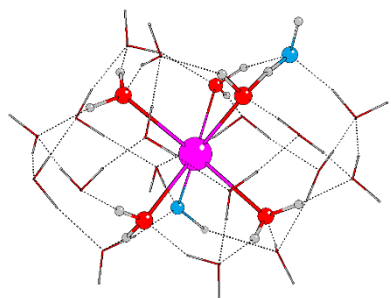


SCF Energy = -1864.3808332762

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -1.3024089 | -2.9558172 | -2.0182701 |
| O     | -1.6273328 | -1.6256916 | 0.1762240  |
| Sr    | 0.3516284  | -0.1749316 | 0.1125065  |
| O     | 1.6596604  | -1.7116490 | 1.5843862  |
| O     | -0.0996111 | 1.6208307  | 1.7915741  |
| O     | -2.4131276 | 2.4544086  | 1.3855806  |
| O     | 1.9242216  | 3.1529259  | 1.3531933  |
| O     | 3.3588827  | -2.5265566 | -0.1157152 |
| O     | 2.5960465  | -0.4158654 | 3.5573384  |
| O     | -1.0279110 | -2.9074621 | 2.3115122  |
| O     | 1.1788988  | 1.7413984  | -1.2172073 |
| O     | 1.2869163  | -1.8699812 | -1.7805910 |
| O     | -2.4914497 | -1.2389207 | -3.6415316 |
| O     | -3.8005287 | 0.5665253  | 2.6237903  |
| O     | 1.9829737  | -0.5909272 | -4.0474208 |
| O     | 3.3614770  | 1.1723997  | -2.5016733 |
| O     | 4.7369301  | -0.0981713 | -0.3585434 |
| O     | -4.5185776 | -0.8809020 | 0.4429704  |
| O     | -0.4953260 | 0.5302481  | -4.5830924 |

|   |            |            |            |
|---|------------|------------|------------|
| O | -0.6320319 | 2.6173562  | -2.8663237 |
| O | -2.9884559 | 2.6036466  | -1.3514203 |
| O | -4.2773384 | 0.2653693  | -2.0791350 |
| O | -1.9933782 | -1.0815677 | 4.1141460  |
| O | 3.9550452  | 1.3542002  | 1.8861247  |
| O | 0.1801272  | 0.6110431  | 4.5355005  |
| H | -0.3353708 | -2.7873232 | -2.1034946 |
| H | -1.5045771 | -2.4762711 | -1.1209594 |
| H | -2.0395794 | -1.9424793 | -3.0618316 |
| H | -2.9546376 | -1.7259760 | -4.3426036 |
| H | -3.6508713 | -0.2961933 | -2.6023529 |
| H | -4.3982822 | -0.1979393 | -1.2150214 |
| H | -2.5659856 | -1.3665896 | 0.2518698  |
| H | -1.4723469 | 2.6118773  | -2.3397708 |
| H | 0.0911957  | 2.3077391  | -2.2015474 |
| H | -0.5894606 | 1.3077988  | -3.9529878 |
| H | -1.1844098 | -0.1140692 | -4.2883583 |
| H | 1.1117390  | -0.1497537 | -4.2514020 |
| H | 2.5295570  | 0.0898614  | -3.5536299 |
| H | 1.5865342  | -1.4514239 | -2.6441637 |
| H | 1.4163079  | 2.4376243  | -0.5775379 |
| H | 3.7696274  | -3.3824204 | 0.0837999  |
| H | 2.6901368  | -2.3051450 | 0.6616811  |
| H | 1.8890966  | 3.9517777  | 1.9030448  |
| H | 1.0793788  | 2.5955096  | 1.5893037  |
| H | 3.2551420  | 2.0364446  | 1.6970241  |
| H | 3.5265735  | 0.7314283  | 2.5299193  |
| H | 4.3253095  | -0.9924503 | -0.2562112 |
| H | 4.4336293  | 0.4188097  | 0.4360388  |
| H | 3.8896322  | 0.6909234  | -1.8171437 |
| H | 2.5040484  | 1.4376222  | -1.9889107 |
| H | 2.2263382  | -1.0154978 | 2.7742728  |
| H | 3.1386602  | -0.9938323 | 4.1175381  |
| H | -0.5449057 | -0.0545249 | 4.4021190  |
| H | 1.0227441  | 0.1681278  | 4.2633128  |
| H | -1.3847432 | 2.1358119  | 1.5866793  |
| H | -0.0484535 | 1.3383240  | 2.7317579  |
| H | 0.9888012  | -2.3485267 | 1.8994772  |
| H | -2.5115854 | 3.3413747  | 1.7683881  |
| H | -1.4402912 | -3.7859846 | 2.3144317  |
| H | -1.3254777 | -2.4450366 | 1.4193632  |
| H | -3.3091700 | 1.3463110  | 2.1994443  |
| H | -4.5121894 | 0.9533497  | 3.1596820  |
| H | -2.6149595 | -0.5146709 | 3.5985507  |
| H | -1.6836416 | -1.7799963 | 3.4721873  |
| H | -4.3644968 | -0.3628703 | 1.2818662  |
| H | -5.0818782 | -1.6333327 | 0.6827333  |
| H | 2.0908395  | -2.2649250 | -1.3541641 |
| H | -2.7787747 | 2.5342371  | -0.3835771 |
| H | -3.4445549 | 1.7530219  | -1.5920229 |

**5 Transition state for the Sr<sup>2+</sup> dihydroxide ([Sr:4/18:2/0]) → Sr<sup>2+</sup> monohydroxide ([Sr:5/17:1/1]) reaction**



SCF Energy = -1865.3263494039

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| O     | -0.5790432 | 2.3401857  | -1.0245693 |
| Sr    | -0.9824667 | 3.4656450  | 1.3199584  |
| O     | 1.5022349  | 3.3914149  | 1.3596560  |
| O     | 1.9565439  | 3.2404321  | -1.1381066 |
| O     | 2.7264867  | 5.4256315  | 2.2994586  |
| O     | -0.8591486 | 5.2826239  | 3.2181599  |
| O     | -2.9299180 | 4.2603116  | 4.4925783  |
| O     | -3.3359147 | 3.4006241  | 2.2489891  |
| O     | -1.8033891 | 2.2666459  | 5.7592977  |
| O     | -0.8215151 | 0.9586610  | 2.1346807  |
| O     | -1.8955521 | 5.5210226  | -0.0516049 |
| O     | -2.0763120 | 3.1679697  | -3.0501351 |
| O     | -0.9034466 | 7.4266025  | 1.5980425  |
| O     | -2.4577511 | 0.2056591  | 4.1353596  |
| O     | -1.0411134 | 5.7599488  | -2.5795132 |
| O     | 1.5242610  | 5.8638001  | -1.9132234 |
| O     | -1.3123913 | -0.1493928 | -0.3042498 |
| O     | 1.3649723  | 5.2137291  | 4.6952927  |
| O     | -4.4598764 | 2.7431619  | -1.7999765 |
| O     | -4.5639289 | 4.8614267  | 0.0444103  |
| O     | -4.5329116 | 1.0193707  | 2.2813653  |
| O     | 1.6713380  | 1.0599515  | 3.2816784  |
| O     | 1.0127076  | 2.6044692  | 5.5152856  |
| O     | -4.1205934 | 0.4048193  | -0.3546095 |
| O     | 1.7182405  | 7.2456047  | 0.4733767  |
| H     | -3.2443333 | 3.8620127  | 3.4145549  |
| H     | -1.6478937 | 5.0701971  | 3.8119734  |
| H     | -0.9268751 | 6.7787187  | 2.3600224  |
| H     | -1.6551853 | 6.3503116  | 0.4461867  |
| H     | -3.6670199 | 5.2771398  | -0.0487908 |
| H     | -3.9366443 | 3.9648482  | 1.7210464  |
| H     | -0.9307714 | 0.6596881  | -0.7465923 |
| H     | 0.3788102  | 2.5374900  | -1.2341001 |
| H     | 1.9051567  | 3.2586217  | -0.0899091 |
| H     | 1.8323402  | 2.6261877  | 1.8672486  |
| H     | 0.8055702  | 0.8441709  | 2.8457756  |
| H     | -0.9522080 | 0.3710436  | 1.3418359  |
| H     | -4.5899839 | 3.4769919  | -1.1508309 |
| H     | -2.9865938 | 3.0854158  | -2.6413916 |
| H     | -4.3405532 | 1.9168636  | -1.2546969 |
| H     | -5.2067980 | 5.5824996  | -0.0543895 |
| H     | -1.8410412 | 4.1247240  | -3.0375550 |
| H     | -1.1161272 | 2.6252528  | -1.8346857 |
| H     | -3.1830680 | 0.1115116  | -0.4145438 |
| H     | -0.8582317 | -0.9184975 | -0.6855143 |
| H     | -0.0448941 | 5.8372445  | -2.4061244 |
| H     | -1.6234096 | 5.6823090  | -1.0042378 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -1.3039200 | 6.5551039  | -3.0711359 |
| H | 1.7709371  | 4.9299462  | -1.6812937 |
| H | 2.7415260  | 2.7274881  | -1.3879577 |
| H | 1.5917259  | 6.3701867  | -1.0560606 |
| H | 0.8272261  | 7.4299311  | 0.8503403  |
| H | 2.1442123  | 6.6361880  | 1.1351939  |
| H | 2.2806304  | 4.5641266  | 1.8997902  |
| H | 1.9994271  | 5.2592577  | 3.9324049  |
| H | 3.6866974  | 5.2893540  | 2.2518444  |
| H | -1.3570537 | 8.2312320  | 1.8975003  |
| H | -4.1087262 | 1.9382632  | 2.2795625  |
| H | -4.2685663 | 0.5724266  | 0.6196929  |
| H | -3.9805657 | 0.5264475  | 2.9239602  |
| H | -2.2629411 | 0.8948910  | 4.8361758  |
| H | -0.0439873 | 5.2912070  | 3.8146825  |
| H | 1.3354984  | 4.2608642  | 4.9858187  |
| H | 1.2629521  | 1.9984957  | 4.7728803  |
| H | 2.1266690  | 0.2107240  | 3.4025862  |
| H | -1.4287233 | 0.6065110  | 2.8501983  |
| H | -2.2769623 | -0.6582585 | 4.5401873  |
| H | -2.2982446 | 3.0667635  | 5.3613340  |
| H | -3.6660180 | 4.7504582  | 4.8905194  |
| H | 0.0384391  | 2.4851534  | 5.6330174  |
| H | -2.0908143 | 2.1995568  | 6.6847264  |

## 6 The effect of infinite permittivity on the relative energies

**Table (i):** Dependence of the absolute and relative SCF and Gibbs free energies on the dielectric constant ( $\epsilon$ ) of the COSMO calculation.

| TOTAL<br>NUMBER<br>OF OH | TYPE OF HYDROXIDE               | $\epsilon=80$     | $\epsilon=\infty$ | $\epsilon=80$     | $\epsilon=\infty$ | $\epsilon=80$            | $\epsilon=\infty$ | $\epsilon=80$          | $\epsilon=\infty$ |
|--------------------------|---------------------------------|-------------------|-------------------|-------------------|-------------------|--------------------------|-------------------|------------------------|-------------------|
|                          |                                 | SCF ENERGY (a.u.) |                   | E+G ENERGY (a.u.) |                   | $\Delta$ SCF<br>(KJ/MOL) |                   | $\Delta$ G<br>(KJ/MOL) |                   |
|                          |                                 |                   |                   |                   |                   |                          |                   |                        |                   |
| 2                        | mono [Sr:5/17:1/1]              | -1865.326         | -1865.328         | -1864.848         | -1864.850         | 0.0                      | 0.0               | 0.0                    | 0.0               |
|                          | di [Sr:4/18:2/0]                | -1865.325         | -1865.327         | -1864.847         | -1864.849         | 3.2                      | 3.0               | 3.1                    | 2.9               |
| 3                        | mono [Sr:5/16:1/2] <sup>-</sup> | -1864.858         | -1864.860         | -1864.392         | -1864.395         | 2.8                      | 2.8               | 3.4                    | 2.9               |
|                          | di [Sr:4/17:2/1] <sup>-</sup>   | -1864.859         | -1864.861         | -1864.394         | -1864.396         | 0.0                      | 0.0               | 0.0                    | 0.0               |
|                          | tri [Sr:3/18:3/0] <sup>-</sup>  | -1864.857         | -1864.859         | -1864.393         | -1864.396         | 5.4                      | 5.1               | 2.4                    | 1.8               |

## 7 Single point calculations for Equation 1 with different basis sets

**Table (ii):** Dependence of SCF energies (kJ/mol) for Equation 1 on basis set quality. For the def2-SVP and def2-TZVP basis sets the error percentages compared with the def2-QZVP are shown in parentheses.

| TOTAL<br>NUMBER<br>OF OH | TYPE OF HYDROXIDE                 | SVP (EQZVP-SVP) |         | TZVP (EQZVP-TZVP) |        | QZVP  |
|--------------------------|-----------------------------------|-----------------|---------|-------------------|--------|-------|
| 1                        | mono [Sr:5/18:1/0] <sup>+</sup>   | -49.3           | (5.3%)  | -36.3             | (1.0%) | -33.3 |
| 2                        | mono [Sr:5/17:1/1]                | -89.1           | (18.8%) | -60.9             | (3.3%) | -54.8 |
|                          | di [Sr:4/18:2/0]                  | -80.3           | (14.7%) | -57.9             | (3.0%) | -52.0 |
| 3                        | mono [Sr:5/16:1/2] <sup>-</sup>   | -115.2          | (32.6%) | -74.5             | (6.1%) | -65.2 |
|                          | di [Sr:4/17:2/1] <sup>-</sup>     | -114.6          | (31.7%) | -77.3             | (6.3%) | -67.9 |
|                          | tri [Sr:3/18:3/0] <sup>-</sup>    | -104.8          | (26.3%) | -72.2             | (5.9%) | -62.9 |
| 4                        | di [Sr:3/17:2/2] <sup>2-</sup>    | -71.4           | (12.3%) | -49.2             | (3.0%) | -42.1 |
|                          | tri [Sr:2/18:3/1] <sup>2-</sup>   | -79.2           | (13.9%) | -60.1             | (3.8%) | -53.0 |
|                          | tetra [Sr:1/19:4/0] <sup>2-</sup> | -72.6           | (11.2%) | -57.6             | (3.6%) | -50.4 |