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An ab initio study of the hydrolysis reactions of neutral and anionic Mg-pyrophosphate complexes in the gas phase

Humberto Saint-Martin and Luis E. Vicent

Supporting Information for the article in J. Phys. Chem. A

The following tables have the cartesian coordinates of all the 23 (twenty three) structures in Å, in the first four columns. The next three columns are the charges obtained from Mulliken's analysis (Mulliken) and from the Chelp method with two ionic radii for the Mg ion; $r = 0.71 \text{ \AA}$ (Chelp1) and $r = 1.70 \text{ \AA}$ (Chelp2) (the radii of the other elements are: $r_H = 1.19 \text{ \AA}$, $r_O = 1.55 \text{ \AA}$ and $r_P = 2.05 \text{ \AA}$). Then the six lowest harmonic frequencies, in cm^{-1} , and finally the SCF/6-31+G** and MP2/6-31+G** energies in atomic units.

Table 1: $Mg \cdot H_2P_2O_7$ structure 1a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -0.168189 | -0.950221 | -0.517065 | -1.385762 | -0.872937 | -0.861920 |
| P ₂ | 1.448728 | -0.493692 | -0.049790 | 2.747981 | 2.066285 | 2.007685 |
| P ₃ | -1.384625 | -0.115351 | -0.063557 | 2.813568 | 1.963302 | 1.947763 |
| O ₄ | 1.712283 | 0.662478 | -1.026848 | -1.046539 | -1.117020 | -1.084047 |
| O ₅ | -1.161155 | 1.364707 | -0.189229 | -1.047761 | -1.046183 | -1.030653 |
| O ₆ | 2.245802 | -1.697044 | -0.007882 | -0.898370 | -0.882735 | -0.870076 |
| O ₇ | -1.748831 | -0.542461 | 1.399032 | -0.914966 | -0.801190 | -0.793366 |
| Mg ₈ | 0.690497 | 1.858587 | 0.081984 | 0.988217 | 1.666307 | 1.624272 |
| O ₉ | -2.616228 | -0.530322 | -0.919179 | -0.867560 | -0.691591 | -0.687900 |
| O ₁₀ | 1.050720 | 0.295529 | 1.229563 | -1.255465 | -1.226296 | -1.185770 |
| H ₁₁ | -2.772717 | -1.460730 | -1.007474 | 0.415027 | 0.435140 | 0.434319 |
| H ₁₂ | -0.990012 | -0.527997 | 1.976717 | 0.451630 | 0.506918 | 0.499693 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|----------|----------|----------|----------|----------|
| 98.9191 | 158.0089 | 194.6450 | 230.6085 | 281.3326 | 301.9562 |
|---------|----------|----------|----------|----------|----------|

$$E(RHF) = -1406.59655280, \Delta E(MP2) = -1.524390400$$

Table 2: $Mg \cdot H_2P_2O_7$ structure 1b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 0.136920 | -1.015645 | -0.033642 | -1.356224 | -0.941990 | -0.936385 |
| P ₂ | -1.326919 | -0.410574 | 0.014694 | 2.868143 | 2.285598 | 2.240501 |
| P ₃ | 1.542724 | -0.135891 | -0.113303 | 2.567647 | 2.131864 | 2.133443 |
| O ₄ | -1.464157 | 0.504612 | 1.206997 | -1.068470 | -1.157593 | -1.127534 |
| O ₅ | 1.094627 | 1.319287 | -0.055610 | -1.056538 | -1.203171 | -1.194522 |
| O ₆ | -2.268162 | -1.651294 | 0.074653 | -0.844121 | -0.747896 | -0.744471 |
| O ₇ | 2.360131 | -0.624308 | -1.208152 | -0.928333 | -0.946369 | -0.947298 |
| Mg ₈ | -0.691057 | 1.908406 | -0.011139 | 0.971287 | 1.725371 | 1.691582 |
| O ₉ | 2.173063 | -0.440404 | 1.309061 | -0.922049 | -0.751611 | -0.752505 |
| O ₁₀ | -1.498732 | 0.500807 | -1.183639 | -1.052556 | -1.213810 | -1.184065 |
| H ₁₁ | 2.856317 | -1.093070 | 1.263168 | 0.408707 | 0.391486 | 0.392124 |
| H ₁₂ | -2.070229 | -2.355259 | -0.527696 | 0.412507 | 0.428121 | 0.429130 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|----------|----------|----------|----------|----------|
| 53.7380 | 145.5527 | 158.7229 | 238.3729 | 262.0970 | 269.8064 |
|---------|----------|----------|----------|----------|----------|

$$E(RHF) = -1406.60291762, \Delta E(MP2) = -1.519810324$$

Table 3: $H_2O \cdot Mg \cdot H_2P_2O_7$ structure 2a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 1.159664 | 0.724465 | -0.497882 | -1.394086 | -0.746040 | -0.727848 |
| P ₂ | -0.291122 | 1.577996 | -0.038192 | 2.803164 | 2.008051 | 1.881115 |
| P ₃ | 1.348320 | -0.744937 | -0.063369 | 2.818169 | 1.668047 | 1.676349 |
| O ₄ | -1.288565 | 1.030216 | -1.063884 | -1.065608 | -1.114621 | -1.021940 |
| O ₅ | 0.132165 | -1.593339 | -0.270997 | -1.083159 | -0.924485 | -0.872511 |
| O ₆ | 0.047757 | 2.981139 | 0.060512 | -0.921093 | -0.897220 | -0.879420 |
| O ₇ | 1.839870 | -0.750378 | 1.427010 | -0.921785 | -0.685770 | -0.670035 |
| Mg ₈ | -1.537711 | -0.582785 | -0.001361 | 0.928080 | 1.658014 | 1.461319 |
| O ₉ | 2.545245 | -1.335225 | -0.872274 | -0.875552 | -0.643853 | -0.669042 |
| O ₁₀ | -0.622463 | 0.716837 | 1.209481 | -1.281182 | -1.158517 | -1.052298 |
| H ₁₁ | 3.320073 | -0.792070 | -0.916691 | 0.412537 | 0.398521 | 0.407002 |
| H ₁₂ | 1.267624 | -0.223076 | 1.979708 | 0.454952 | 0.427663 | 0.400203 |
| O ₁₃ | -3.164596 | -1.799275 | 0.065344 | -0.742106 | -0.971092 | -0.877679 |
| H ₁₄ | -4.070139 | -1.536846 | -0.031559 | 0.436038 | 0.497742 | 0.484500 |
| H ₁₅ | -3.115626 | -2.746005 | 0.049799 | 0.431630 | 0.483560 | 0.460285 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|----------|----------|----------|----------|
| 25.6338 | 50.2990 | 114.2886 | 152.7134 | 161.5062 | 197.7506 |
|---------|---------|----------|----------|----------|----------|

$$E(RHF) = -1482.68297689, \Delta E(MP2) = -1.7268830062$$

Table 4: $H_2O \cdot Mg \cdot H_2P_2O_7$ structure 2b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -1.187361 | 0.754092 | -0.071255 | -1.399201 | -0.923300 | -0.890884 |
| P ₂ | 0.229466 | 1.471139 | -0.002924 | 2.940736 | 2.084189 | 2.032627 |
| P ₃ | -1.419659 | -0.885334 | -0.122340 | 2.588927 | 1.954208 | 1.884350 |
| O ₄ | 0.969726 | 0.964716 | 1.212270 | -1.072436 | -1.072814 | -1.020291 |
| O ₅ | -0.022239 | -1.477345 | -0.104396 | -1.134431 | -1.096075 | -1.023026 |
| O ₆ | -0.129192 | 2.993153 | -0.001114 | -0.874528 | -0.839947 | -0.850895 |
| O ₇ | -2.364842 | -1.213834 | -1.175725 | -0.925147 | -0.874750 | -0.866469 |
| Mg ₈ | 1.627566 | -0.518008 | -0.015873 | 0.916221 | 1.601480 | 1.467401 |
| O ₉ | -2.025772 | -1.154265 | 1.324148 | -0.927862 | -0.674789 | -0.681031 |
| O ₁₀ | 1.074367 | 1.054340 | -1.178008 | -1.061632 | -1.029660 | -0.975728 |
| H ₁₁ | -2.962494 | -1.279444 | 1.288211 | 0.405255 | 0.326363 | 0.338144 |
| H ₁₂ | -0.961194 | 3.218607 | 0.389932 | 0.416463 | 0.502380 | 0.506328 |
| O ₁₃ | 3.104189 | -1.902000 | 0.032069 | -0.750361 | -0.891163 | -0.819515 |
| H ₁₄ | 4.047650 | -1.845218 | 0.083947 | 0.441783 | 0.468584 | 0.452283 |
| H ₁₅ | 2.847143 | -2.815764 | 0.003419 | 0.436212 | 0.465295 | 0.446707 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|----------|----------|
| 32.1338 | 44.9728 | 48.0032 | 62.7619 | 145.2238 | 170.1179 |
|---------|---------|---------|---------|----------|----------|

$$E(RHF) = -1482.69022174, \Delta E(MP2) = -1.722373193$$

Table 5: $PO_3 \cdot Mg \cdot H_2PO_4$ structure 3

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mg ₁ | 0.302291 | -0.045427 | 0.019805 | 0.770017 | 1.645374 | 1.541164 |
| P ₂ | -2.231757 | -0.003274 | 0.017632 | 2.611938 | 1.807229 | 1.724768 |
| P ₃ | 2.876655 | 0.005201 | -0.006905 | 1.995643 | 1.912831 | 1.865084 |
| O ₄ | -1.309222 | -0.044263 | 1.205644 | -0.980043 | -1.018316 | -0.965159 |
| O ₅ | -1.304908 | 0.076633 | -1.175445 | -1.009124 | -1.055255 | -0.999407 |
| O ₆ | 1.994165 | -1.195582 | -0.052873 | -0.778761 | -1.003113 | -0.951460 |
| O ₇ | 1.954077 | 1.174171 | 0.058276 | -0.782660 | -1.011071 | -0.964172 |
| O ₈ | -3.176804 | -1.253304 | 0.028322 | -0.877208 | -0.703141 | -0.682594 |
| O ₉ | -3.275060 | 1.180216 | 0.015108 | -0.878521 | -0.698987 | -0.681624 |
| O ₁₀ | 4.308340 | 0.030098 | -0.023700 | -0.886047 | -0.737990 | -0.736045 |
| H ₁₁ | -3.886873 | -1.253311 | -0.597055 | 0.406338 | 0.440405 | 0.432513 |
| H ₁₂ | -2.938789 | 2.025789 | -0.244167 | 0.408428 | 0.422034 | 0.416933 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|----------|----------|----------|
| 47.7600 | 56.2973 | 58.5108 | 156.8280 | 180.3809 | 191.6496 |
|---------|---------|---------|----------|----------|----------|

$$E(RHF) = -1406.61483160, \Delta E(MP2) = -1.526764900$$

Table 6: $H_2O \cdot PO_3 \cdot Mg \cdot H_2PO_4$ structure 4a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 1.644191 | -0.054848 | 1.211832 | -0.987732 | -0.894101 | -0.861718 |
| P ₂ | -3.097892 | -0.357745 | 0.003288 | 1.941320 | 1.903786 | 1.898318 |
| P ₃ | 2.523632 | -0.184720 | 0.000722 | 2.638365 | 1.481850 | 1.545735 |
| O ₄ | -3.297297 | 1.093265 | -0.025861 | -0.946143 | -0.837809 | -0.848535 |
| O ₅ | 1.630928 | -0.051910 | -1.200394 | -0.998805 | -0.903594 | -0.874914 |
| O ₆ | -1.655627 | -0.770005 | 0.026005 | -0.855453 | -1.044656 | -0.980308 |
| O ₇ | 3.296472 | -1.560643 | 0.044647 | -0.882078 | -0.689890 | -0.724435 |
| Mg ₈ | 0.019183 | 0.176726 | 0.017925 | 0.846126 | 1.653849 | 1.528510 |
| O ₉ | 3.648892 | 0.923795 | -0.057007 | -0.872935 | -0.692119 | -0.707440 |
| O ₁₀ | -4.131728 | -1.359309 | 0.010117 | -0.825332 | -0.841925 | -0.853909 |
| H ₁₁ | 4.204537 | 0.981068 | 0.707175 | 0.407720 | 0.466495 | 0.462034 |
| H ₁₂ | 3.650093 | -1.856740 | -0.781992 | 0.412888 | 0.458050 | 0.457062 |
| O ₁₃ | -0.792662 | 2.026405 | -0.016800 | -0.804041 | -1.016149 | -1.087415 |
| H ₁₄ | -1.759160 | 2.014538 | -0.028387 | 0.499658 | 0.487986 | 0.548551 |
| H ₁₅ | -0.457138 | 2.903403 | -0.112360 | 0.426444 | 0.468227 | 0.498463 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|----------|----------|
| 35.5275 | 40.6181 | 45.2590 | 77.5083 | 128.2062 | 140.7161 |
|---------|---------|---------|---------|----------|----------|

 $E(RHF) = -1482.68156723$, $\Delta E(MP2) = -1.727644388$

Table 7: $H_2O \cdot PO_3 \cdot Mg \cdot H_2PO_4$ structure 4b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 1.127188 | -0.525705 | 1.071782 | -0.998725 | -0.984677 | -0.962303 |
| P ₂ | -2.756854 | -0.395501 | 0.049894 | 2.012447 | 1.710443 | 1.690149 |
| P ₃ | 2.199034 | -0.286112 | 0.038572 | 2.598516 | 1.626683 | 1.668007 |
| O ₄ | -2.142394 | 0.619963 | 0.942858 | -0.819803 | -0.847383 | -0.817459 |
| O ₅ | 1.531489 | 0.438942 | -1.090477 | -1.016792 | -0.889700 | -0.877074 |
| O ₆ | -4.110631 | -0.871402 | 0.099264 | -0.892177 | -0.736792 | -0.737654 |
| O ₇ | 2.915518 | -1.638173 | -0.365170 | -0.880247 | -0.664514 | -0.681250 |
| Mg ₈ | -0.275042 | 0.408586 | -0.059359 | 0.722961 | 1.554876 | 1.444038 |
| O ₉ | 3.420248 | 0.557627 | 0.565677 | -0.882382 | -0.719325 | -0.739918 |
| O ₁₀ | -1.709304 | -0.818948 | -0.917960 | -0.768036 | -0.921769 | -0.891682 |
| H ₁₁ | 3.969362 | 0.131075 | 1.207127 | 0.403416 | 0.462634 | 0.463720 |
| H ₁₂ | 2.335868 | -2.375814 | -0.489316 | 0.406879 | 0.397589 | 0.399762 |
| O ₁₃ | -0.307654 | 2.441225 | -0.374565 | -0.743094 | -0.960429 | -0.880059 |
| H ₁₄ | -0.864729 | 3.092762 | 0.023739 | 0.426270 | 0.468458 | 0.439461 |
| H ₁₅ | 0.431622 | 2.844905 | -0.807485 | 0.430766 | 0.503906 | 0.482263 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|----------|----------|
| 35.4362 | 40.4525 | 45.3415 | 77.5120 | 128.2115 | 140.6924 |
|---------|---------|---------|---------|----------|----------|

$$E(RHF) = -1482.67988460, \Delta E(MP2) = -1.731841724$$

Table 8: $H_2PO_4 \cdot Mg \cdot H_2PO_4$ structure 5

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mg ₁ | -0.000025 | -0.013480 | 0.033790 | 0.657874 | 1.685737 | 1.453194 |
| P ₂ | 2.540968 | 0.023551 | -0.009508 | 2.610683 | 1.884083 | 1.877730 |
| P ₃ | -2.541209 | -0.021085 | -0.009081 | 2.611292 | 1.895121 | 1.887783 |
| O ₄ | 1.652485 | -0.860697 | 0.833033 | -1.007000 | -1.116671 | -1.020930 |
| O ₅ | -1.643568 | 0.853691 | 0.833050 | -1.007074 | -1.119061 | -1.021930 |
| O ₆ | 1.605650 | 0.836058 | -0.857745 | -0.982497 | -1.052196 | -0.983998 |
| O ₇ | -1.614300 | -0.849146 | -0.852027 | -0.982073 | -1.052609 | -0.983978 |
| O ₈ | 3.481215 | 0.974249 | 0.814721 | -0.877557 | -0.683705 | -0.697733 |
| O ₉ | -3.496670 | -0.956908 | 0.814721 | -0.877219 | -0.688495 | -0.700536 |
| O ₁₀ | 3.597328 | -0.836561 | -0.813860 | -0.881197 | -0.691685 | -0.702310 |
| O ₁₁ | -3.583325 | 0.850278 | -0.819878 | -0.881689 | -0.698770 | -0.708307 |
| H ₁₂ | 4.177406 | 0.554597 | 1.298513 | 0.402582 | 0.418804 | 0.409378 |
| H ₁₃ | -4.189561 | -0.526747 | 1.293997 | 0.402528 | 0.420088 | 0.408138 |
| H ₁₄ | 3.267849 | -1.651018 | -1.164928 | 0.405577 | 0.398162 | 0.390722 |
| H ₁₅ | -3.242285 | 1.660244 | -1.170346 | 0.405770 | 0.401195 | 0.392775 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|----------|----------|----------|
| 47.0372 | 47.1645 | 55.8107 | 156.5194 | 158.9895 | 179.6677 |
|---------|---------|---------|----------|----------|----------|

 $E(RHF) = -1482.72630448$, $\Delta E(MP2) = -1.715369756$ Table 9: $[Mg \cdot HP_2O_7]^-$ structure 6a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 0.132808 | -0.955326 | -0.146209 | -1.434831 | -1.019533 | -0.989174 |
| P ₂ | -1.464185 | -0.482092 | -0.005658 | 2.855833 | 2.404818 | 2.285632 |
| P ₃ | 1.509910 | -0.151956 | -0.129659 | 2.660190 | 2.328160 | 2.284348 |
| O ₄ | -1.412685 | 0.464855 | 1.226210 | -1.167234 | -1.298284 | -1.219869 |
| O ₅ | 1.175932 | 1.346386 | -0.088114 | -1.110258 | -1.273328 | -1.205723 |
| O ₆ | -1.579526 | 0.570449 | -1.144834 | -1.135517 | -1.338729 | -1.262723 |
| O ₇ | 2.440771 | -0.639666 | -1.149365 | -1.002091 | -1.062271 | -1.059928 |
| Mg ₈ | -0.645733 | 1.786225 | 0.035640 | 0.871201 | 1.735386 | 1.622812 |
| O ₉ | 2.103833 | -0.453051 | 1.335893 | -0.945525 | -0.820169 | -0.829173 |
| O ₁₀ | -2.308943 | -1.670895 | 0.002631 | -0.974318 | -1.024448 | -1.004366 |
| H ₁₁ | 2.645398 | -1.225990 | 1.312360 | 0.382551 | 0.368399 | 0.378165 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|----------|----------|----------|----------|----------|
| 52.6500 | 141.4586 | 216.8834 | 222.6025 | 292.3443 | 299.8214 |
|---------|----------|----------|----------|----------|----------|

 $E(RHF) = -1406.08247680$, $\Delta E(MP2) = -1.534602581$

Table 10: $[Mg \cdot HP_2O_7]^-$ structure 6b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -0.116685 | -0.918707 | -0.500532 | -1.468427 | -0.987298 | -0.952627 |
| P ₂ | -1.510088 | -0.198010 | -0.134608 | 2.735599 | 2.301340 | 2.246642 |
| P ₃ | 1.414991 | -0.459425 | -0.057939 | 2.857890 | 2.236945 | 2.140081 |
| O ₄ | -1.665354 | -0.538247 | 1.423201 | -0.963329 | -0.909486 | -0.892659 |
| O ₅ | 2.302430 | -1.615337 | -0.027297 | -0.966645 | -0.999254 | -0.982613 |
| O ₆ | -1.243104 | 1.324709 | -0.209890 | -1.108845 | -1.262508 | -1.204919 |
| O ₇ | 1.101025 | 0.329961 | 1.258263 | -1.287059 | -1.269101 | -1.202147 |
| Mg ₈ | 0.551955 | 1.797677 | 0.076581 | 0.877718 | 1.651646 | 1.562057 |
| O ₉ | -2.629522 | -0.720025 | -0.906377 | -1.004410 | -1.018397 | -1.013403 |
| O ₁₀ | 1.706458 | 0.723249 | -1.025238 | -1.102432 | -1.204665 | -1.148857 |
| H ₁₁ | -0.838992 | -0.395409 | 1.872195 | 0.429940 | 0.460780 | 0.448445 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|----------|----------|----------|----------|----------|
| 98.5373 | 147.8790 | 221.4400 | 293.0742 | 305.6780 | 312.6107 |
|---------|----------|----------|----------|----------|----------|

$$E(RHF) = -1406.08662518, \Delta E(MP2) = -1.537385186$$

Table 11: $[H_2O \cdot Mg \cdot HP_2O_7]^-$ structure 7

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 0.527058 | -1.241303 | -0.362315 | -1.460849 | -0.811807 | -0.777002 |
| P ₂ | -1.059883 | -1.173583 | -0.126251 | 2.768571 | 2.040055 | 2.007910 |
| P ₃ | 1.643151 | -0.065008 | 0.007112 | 2.858022 | 1.824095 | 1.708161 |
| O ₄ | -1.171321 | -1.269340 | 1.472178 | -0.972646 | -0.842924 | -0.822850 |
| O ₅ | 2.946108 | -0.677534 | 0.246364 | -0.976507 | -0.879434 | -0.873835 |
| O ₆ | -1.488447 | 0.265904 | -0.486304 | -1.206602 | -1.201417 | -1.112268 |
| O ₇ | 0.900862 | 0.675648 | 1.165524 | -1.298853 | -1.129426 | -1.008720 |
| Mg ₈ | -0.123194 | 1.610592 | -0.257764 | 0.829878 | 1.681605 | 1.384509 |
| O ₉ | -1.773714 | -2.269800 | -0.770209 | -1.016433 | -0.959630 | -0.968733 |
| O ₁₀ | 1.467198 | 0.957393 | -1.146321 | -1.095508 | -1.132190 | -1.009547 |
| H ₁₁ | -0.513284 | -0.705718 | 1.867770 | 0.435887 | 0.411565 | 0.389139 |
| O ₁₂ | -1.724394 | 2.869738 | 0.131722 | -0.739552 | -0.960636 | -0.768333 |
| H ₁₃ | -2.334618 | 2.132650 | 0.072770 | 0.462307 | 0.519360 | 0.453199 |
| H ₁₄ | -1.889583 | 3.339177 | 0.934610 | 0.412285 | 0.440784 | 0.398368 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|----------|----------|----------|----------|
| 42.7340 | 98.6219 | 136.4081 | 157.4256 | 225.8419 | 275.6765 |
|---------|---------|----------|----------|----------|----------|

$$E(RHF) = -1482.16217805, \Delta E(MP2) = -1.742074834$$

Table 12: $[PO_3 \cdot Mg \cdot HPO_4]^-$ structure 8

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mg ₁ | -0.211173 | -0.047854 | 0.000405 | 0.759689 | 1.652366 | 1.511090 |
| P ₂ | 2.305385 | -0.108979 | -0.000113 | 2.616141 | 2.422191 | 2.365461 |
| P ₃ | -2.836998 | 0.015914 | -0.000099 | 1.956988 | 1.975365 | 1.925383 |
| O ₄ | 1.304871 | -0.081963 | 1.189696 | -1.081510 | -1.258383 | -1.202085 |
| O ₅ | 1.304402 | -0.083634 | -1.189433 | -1.081830 | -1.257746 | -1.201520 |
| O ₆ | -1.931045 | 1.190152 | 0.000648 | -0.796157 | -1.017136 | -0.955059 |
| O ₇ | -1.989865 | -1.201317 | -0.000295 | -0.790095 | -1.058750 | -0.998677 |
| O ₈ | 3.033322 | 1.346651 | -0.001926 | -0.991974 | -0.877624 | -0.856880 |
| O ₉ | 3.372518 | -1.126948 | 0.000891 | -1.051064 | -1.091069 | -1.082285 |
| O ₁₀ | -4.276553 | 0.051729 | -0.000226 | -0.920195 | -0.811443 | -0.813944 |
| H ₁₁ | 3.967071 | 1.212866 | 0.003475 | 0.380008 | 0.322228 | 0.308516 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|----------|----------|----------|
| 57.3430 | 59.2620 | 60.9005 | 152.7826 | 183.9897 | 196.8253 |
|---------|---------|---------|----------|----------|----------|

$$E(RHF) = -1406.09266000, \Delta E(MP2) = -1.540658198$$

Table 13: $[H_2O \cdot PO_3 \cdot Mg \cdot HPO_4]^-$ structure 9

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -1.495694 | -0.032818 | -1.141196 | -1.101642 | -1.056345 | -1.038744 |
| P ₂ | 3.106030 | -0.256898 | -0.046308 | 1.918380 | 2.011201 | 1.987454 |
| P ₃ | -2.589007 | -0.291037 | -0.071236 | 2.630443 | 1.690700 | 1.709316 |
| O ₄ | 3.167898 | 1.187350 | -0.283884 | -0.946459 | -0.920278 | -0.908877 |
| O ₅ | -1.713383 | -0.448719 | 1.200745 | -1.058575 | -1.048757 | -1.028087 |
| O ₆ | 1.744977 | -0.810242 | 0.208099 | -0.859441 | -1.110675 | -1.055474 |
| O ₇ | -3.627073 | -1.303161 | -0.342226 | -1.047761 | -0.928687 | -0.938665 |
| Mg ₈ | -0.088815 | -0.091548 | 0.206837 | 0.836037 | 1.694603 | 1.599188 |
| O ₉ | -3.355452 | 1.143163 | 0.100738 | -1.018714 | -0.728927 | -0.734896 |
| O ₁₀ | 4.254242 | -1.136794 | -0.039162 | -0.850275 | -0.910535 | -0.914468 |
| H ₁₁ | -4.284433 | 0.994821 | 0.031876 | 0.381519 | 0.368787 | 0.367132 |
| O ₁₂ | 0.545065 | 1.884624 | 0.238841 | -0.768744 | -0.998027 | -0.953916 |
| H ₁₃ | 1.456178 | 2.002542 | -0.029509 | 0.473779 | 0.520648 | 0.500831 |
| H ₁₄ | -0.025929 | 2.453012 | -0.256912 | 0.411454 | 0.416292 | 0.409207 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|----------|----------|
| 35.1251 | 41.3289 | 44.1506 | 73.7226 | 126.8425 | 142.3031 |
|---------|---------|---------|---------|----------|----------|

$$E(RHF) = -1482.15785986, \Delta E(MP2) = -1.742338025$$

Table 14: $[H_2PO_4 \cdot Mg \cdot HPO_4]^-$ structure 10

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mg ₁ | -0.087344 | -0.026848 | -0.042218 | 0.629665 | 1.753723 | 1.463782 |
| P ₂ | 2.510157 | 0.005609 | 0.008547 | 2.617217 | 1.998342 | 2.002736 |
| P ₃ | -2.608958 | -0.058774 | -0.091642 | 2.618309 | 2.248109 | 2.248882 |
| O ₄ | 1.591734 | 0.676481 | 0.985599 | -1.011316 | -1.127928 | -1.024626 |
| O ₅ | -1.618522 | 0.962212 | -0.711890 | -1.083180 | -1.258034 | -1.158515 |
| O ₆ | 1.645437 | -0.687054 | -1.001887 | -1.005047 | -1.164968 | -1.072563 |
| O ₇ | -1.618075 | -1.050072 | 0.574596 | -1.082690 | -1.292762 | -1.189056 |
| O ₈ | 3.534884 | 1.056327 | -0.592027 | -0.904229 | -0.717090 | -0.728521 |
| O ₉ | -3.345825 | 0.726141 | 1.134083 | -0.994008 | -0.846825 | -0.868340 |
| O ₁₀ | 3.537411 | -1.019977 | 0.646799 | -0.904620 | -0.758479 | -0.787306 |
| O ₁₁ | -3.680261 | -0.607795 | -0.948144 | -1.062257 | -1.066599 | -1.095494 |
| H ₁₂ | 3.202709 | 1.940648 | -0.551937 | 0.401934 | 0.402589 | 0.386428 |
| H ₁₃ | -4.277921 | 0.641579 | 1.017963 | 0.378032 | 0.386340 | 0.384447 |
| H ₁₄ | 3.231077 | -1.912671 | 0.589993 | 0.402191 | 0.443583 | 0.438146 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|----------|----------|----------|
| 43.6693 | 57.0253 | 57.5448 | 156.2550 | 169.4018 | 184.4956 |
|---------|---------|---------|----------|----------|----------|

$$E(RHF) = -1482.19307937, \Delta E(MP2) = -1.730596473$$

Table 15: $[Mg \cdot P_2O_7]^{2-}$ structure 11a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 0.063019 | -0.912615 | -0.000280 | -1.484154 | -1.145629 | -1.098928 |
| P ₂ | 1.627846 | -0.239139 | 0.000005 | 2.653062 | 2.389588 | 2.336227 |
| P ₃ | -1.473946 | -0.431053 | 0.000030 | 2.912932 | 2.713645 | 2.571386 |
| O ₄ | 2.250859 | -0.656814 | 1.285266 | -1.119849 | -1.134720 | -1.127645 |
| O ₅ | -1.536681 | 0.587788 | 1.195506 | -1.192320 | -1.415029 | -1.330890 |
| O ₆ | 2.251098 | -0.657041 | -1.285077 | -1.119871 | -1.134745 | -1.127676 |
| O ₇ | -1.537132 | 0.588038 | -1.195253 | -1.192253 | -1.415014 | -1.330875 |
| Mg ₈ | -0.467647 | 1.698589 | -0.000014 | 0.768559 | 1.675661 | 1.556679 |
| O ₉ | -2.412905 | -1.567262 | -0.000023 | -1.055439 | -1.187028 | -1.165864 |
| O ₁₀ | 1.334648 | 1.326633 | -0.000185 | -1.170666 | -1.346728 | -1.282414 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|----------|----------|----------|----------|----------|
| 46.8279 | 129.4872 | 178.4058 | 280.6294 | 291.9868 | 309.7200 |
|---------|----------|----------|----------|----------|----------|

$$E(RHF) = -1405.38792830, \Delta E(MP2) = -1.551949381$$

Table 16: $[Mg \cdot P_2O_7]^{2-}$ structure 11b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 0.000005 | 1.057899 | 0.000228 | -1.353728 | -0.896479 | -0.841286 |
| P ₂ | -1.555611 | 0.316362 | 0.000060 | 2.719209 | 2.011438 | 1.897231 |
| P ₃ | 1.555615 | 0.316382 | -0.000025 | 2.719246 | 2.011690 | 1.897440 |
| O ₄ | -2.595637 | 1.413358 | 0.000642 | -1.059858 | -1.000587 | -0.987714 |
| O ₅ | 1.470591 | -0.694152 | 1.224111 | -1.114270 | -1.190937 | -1.124844 |
| O ₆ | -1.470189 | -0.693950 | -1.224181 | -1.114208 | -1.190824 | -1.124730 |
| O ₇ | 1.469030 | -0.694461 | -1.223690 | -1.114184 | -1.191056 | -1.124854 |
| Mg ₈ | 0.000003 | -1.529273 | -0.000170 | 0.491821 | 1.638470 | 1.521405 |
| O ₉ | 2.595616 | 1.413398 | -0.000780 | -1.059843 | -1.000670 | -0.987782 |
| O ₁₀ | -1.469427 | -0.694576 | 1.223857 | -1.114185 | -1.191042 | -1.124866 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|----------|----------|----------|----------|----------|----------|
| 139.5542 | 193.3293 | 224.2913 | 275.3565 | 282.6154 | 329.6024 |
|----------|----------|----------|----------|----------|----------|

$$E(RHF) = -1405.38342128, \Delta E(MP2) = -1.558244686$$

Table 17: $[H_2O \cdot Mg \cdot P_2O_7]^{2-}$ structure 12a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 0.677092 | 1.015742 | -0.014332 | -1.474752 | -0.955817 | -0.935966 |
| P ₂ | -0.918439 | 1.091637 | 0.000146 | 2.964068 | 2.208245 | 2.166662 |
| P ₃ | 1.902822 | -0.173952 | -0.001669 | 2.658238 | 2.293509 | 2.270908 |
| O ₄ | -1.361456 | 0.161566 | -1.189094 | -1.270826 | -1.249602 | -1.200190 |
| O ₅ | 1.072107 | -1.524754 | 0.001039 | -1.156186 | -1.371475 | -1.299433 |
| O ₆ | -1.417701 | 2.479887 | -0.003001 | -1.039538 | -1.080719 | -1.085402 |
| O ₇ | 2.626031 | 0.009060 | 1.285817 | -1.122006 | -1.129589 | -1.134208 |
| Mg ₈ | -0.761171 | -1.321448 | 0.011570 | 0.665170 | 1.723586 | 1.582065 |
| O ₉ | 2.637403 | -0.002732 | -1.284330 | -1.120226 | -1.130667 | -1.133953 |
| O ₁₀ | -1.343598 | 0.170998 | 1.201070 | -1.270606 | -1.256543 | -1.201126 |
| O ₁₁ | -2.872736 | -1.761694 | -0.012047 | -0.728976 | -1.017122 | -0.926860 |
| H ₁₂ | -2.861590 | -1.127064 | -0.735731 | 0.451951 | 0.486111 | 0.452904 |
| H ₁₃ | -2.907236 | -1.165418 | 0.738762 | 0.443690 | 0.480083 | 0.444600 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|----------|----------|----------|----------|
| 30.1682 | 42.8841 | 128.5694 | 132.2998 | 206.3228 | 254.7379 |
|---------|---------|----------|----------|----------|----------|

$$E(RHF) = -1481.46254399, \Delta E(MP2) = -1.759508383$$

Table 18: $[HO \cdot Mg \cdot HP_2O_7]^{2-}$ structure 12b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -1.057434 | 0.881650 | -0.432040 | -1.466451 | -0.932674 | -0.912204 |
| P ₂ | -1.558452 | -0.614730 | -0.126773 | 2.713725 | 2.238151 | 2.235775 |
| P ₃ | 0.467050 | 1.433102 | -0.037518 | 2.854684 | 1.924820 | 1.837363 |
| O ₄ | -2.843239 | -0.898810 | -0.783182 | -1.078827 | -1.066873 | -1.082888 |
| O ₅ | 0.396153 | 2.900600 | 0.093923 | -1.059391 | -0.987502 | -0.985988 |
| O ₆ | -0.383514 | -1.545371 | -0.386609 | -1.139759 | -1.174425 | -1.119080 |
| O ₇ | 1.376936 | 0.821792 | -1.110518 | -1.126532 | -1.129506 | -1.054355 |
| Mg ₈ | 1.473894 | -0.920032 | -0.073561 | 0.883503 | 1.749439 | 1.555129 |
| O ₉ | -1.769603 | -0.571210 | 1.473817 | -0.997939 | -0.938137 | -0.926001 |
| O ₁₀ | 0.785910 | 0.577955 | 1.214430 | -1.324459 | -1.160124 | -1.072850 |
| O ₁₁ | 2.970869 | -2.077878 | 0.100233 | -1.000882 | -1.310536 | -1.223559 |
| H ₁₂ | -0.968611 | -0.214287 | 1.851273 | 0.440757 | 0.448207 | 0.425504 |
| H ₁₃ | 3.844292 | -1.730736 | 0.135387 | 0.301571 | 0.339160 | 0.323154 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|----------|----------|----------|----------|----------|
| 92.6227 | 124.9318 | 148.6823 | 163.7269 | 210.8855 | 237.3370 |
|---------|----------|----------|----------|----------|----------|

$$E(RHF) = -1481.55370965, \Delta E(MP2) = -1.751050204$$

Table 19: $[PO_3 \cdot Mg \cdot PO_4]^{2-}$ structure 13a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -1.822686 | -0.233469 | 1.372728 | -1.275011 | -1.280908 | -1.239430 |
| P ₂ | -2.593268 | -0.002914 | 0.004703 | 2.698431 | 2.233306 | 2.186980 |
| P ₃ | 3.093210 | -0.002685 | 0.000934 | 1.852313 | 2.214585 | 2.126733 |
| O ₄ | -1.854339 | 1.311920 | -0.485132 | -1.269633 | -1.298851 | -1.265788 |
| O ₅ | 1.610317 | 0.031216 | -0.022980 | -0.893864 | -1.127927 | -1.011235 |
| O ₆ | -4.080768 | -0.015724 | 0.020431 | -1.073620 | -1.067388 | -1.067540 |
| O ₇ | 3.760543 | -1.298067 | 0.010680 | -0.884673 | -1.022389 | -1.003967 |
| Mg ₈ | -0.35239 | 0.013940 | -0.015024 | 1.000537 | 1.672464 | 1.521757 |
| O ₉ | 3.816719 | 1.262378 | 0.011902 | -0.883346 | -1.025121 | -1.004376 |
| O ₁₀ | -1.838587 | -1.068667 | -0.895663 | -1.271134 | -1.297771 | -1.243134 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|--------|---------|---------|----------|----------|----------|
| 2.6246 | 30.7708 | 38.9622 | 116.3910 | 147.1204 | 195.5651 |
|--------|---------|---------|----------|----------|----------|

$$E(RHF) = -1405.37659770, \Delta E(MP2) = -1.555503020$$

Table 20: $[PO_3 \cdot Mg \cdot PO_4]^{2-}$ structure 13b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mg ₁ | 0.207865 | -0.000676 | 0.000735 | 0.827074 | 1.597948 | 1.554745 |
| O ₂ | 1.625218 | 0.000890 | 1.215139 | -1.156657 | -1.374740 | -1.311588 |
| P ₃ | 2.710704 | 0.000140 | -0.000208 | 2.587482 | 2.600745 | 2.305435 |
| O ₄ | 3.490413 | 1.286069 | -0.001648 | -1.165254 | -1.266928 | -1.172130 |
| O ₅ | 1.624390 | -0.001363 | -1.214718 | -1.156717 | -1.374669 | -1.311514 |
| O ₆ | 3.491260 | -1.285285 | 0.000748 | -1.165277 | -1.266986 | -1.173262 |
| O ₇ | -1.741478 | -0.000765 | 0.000670 | -0.861209 | -1.013724 | -0.958954 |
| P ₈ | -3.227613 | 0.000113 | -0.000075 | 1.850673 | 1.990699 | 1.941135 |
| O ₉ | -3.915475 | 1.283336 | -0.000247 | -0.880060 | -0.946169 | -0.936567 |
| O ₁₀ | -3.916922 | -1.282343 | -0.000517 | -0.880055 | -0.946175 | -0.937300 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|----------|----------|
| 21.6249 | 26.9052 | 38.2920 | 64.3652 | 162.1380 | 181.0514 |
|---------|---------|---------|---------|----------|----------|

$$E(RHF) = -1405.37795242, \Delta E(MP2) = -1.554011475$$

Table 21: $[H_2O \cdot PO_3 \cdot Mg \cdot PO_4]^{2-}$ structure 14a

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | -1.615200 | -1.578707 | -0.001945 | -1.248431 | -1.257033 | -1.220700 |
| P ₂ | -2.554891 | -0.316395 | -0.000306 | 2.799639 | 2.351334 | 2.259946 |
| P ₃ | 3.152179 | -0.202932 | -0.000270 | 1.857286 | 2.214947 | 2.129149 |
| O ₄ | -1.920706 | 0.489494 | 1.212271 | -1.323609 | -1.290593 | -1.214964 |
| O ₅ | 1.674239 | -0.306364 | 0.000564 | -0.875423 | -1.144330 | -1.033748 |
| O ₆ | -4.027158 | -0.518302 | -0.000597 | -1.076587 | -1.158682 | -1.153203 |
| O ₇ | 3.849308 | -0.161872 | -1.280535 | -0.889575 | -1.029846 | -1.011362 |
| Mg ₈ | -0.276154 | -0.046605 | 0.000223 | 0.876867 | 1.695161 | 1.539255 |
| O ₉ | 3.850991 | -0.167008 | 1.279251 | -0.889543 | -1.030051 | -1.011627 |
| O ₁₀ | -1.920947 | 0.492568 | -1.210955 | -1.323596 | -1.290270 | -1.214688 |
| O ₁₁ | -0.358671 | 2.277894 | 0.002128 | -0.809389 | -1.049272 | -0.999304 |
| H ₁₂ | -0.949840 | 2.063516 | 0.730906 | 0.451073 | 0.494400 | 0.465713 |
| H ₁₃ | -0.950476 | 2.064019 | -0.726398 | 0.451289 | 0.494235 | 0.465532 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|----------|----------|
| 24.5010 | 25.9111 | 31.2139 | 62.3259 | 122.6341 | 143.3044 |
|---------|---------|---------|---------|----------|----------|

$$E(RHF) = -1481.44375094, \Delta E(MP2) = -1.765804670$$

Table 22: $[HO \cdot PO_3 \cdot Mg \cdot HPO_4]^{2-}$ structure 14b

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| O ₁ | 1.553351 | 0.073134 | 1.177603 | -1.121984 | -1.143542 | -1.070431 |
| P ₂ | -3.066832 | -0.381223 | 0.068130 | 1.838270 | 1.881139 | 1.886894 |
| P ₃ | 2.508062 | -0.431502 | 0.073559 | 2.590580 | 1.723837 | 1.683774 |
| O ₄ | -3.659074 | 0.424812 | 1.134092 | -0.912436 | -0.919784 | -0.918393 |
| O ₅ | 1.667718 | -0.189552 | -1.200229 | -1.113548 | -1.089298 | -1.024751 |
| O ₆ | -1.595369 | -0.443618 | -0.062605 | -0.856175 | -1.011172 | -0.966526 |
| O ₇ | 3.172052 | -1.741339 | 0.250549 | -1.077491 | -0.938678 | -0.947003 |
| Mg ₈ | 0.143294 | 0.611819 | -0.161456 | 0.858304 | 1.795800 | 1.615578 |
| O ₉ | 3.724505 | 0.681588 | 0.007233 | -0.588829 | -0.785055 | -0.783371 |
| O ₁₀ | -3.892345 | -1.154335 | -0.858232 | -0.899611 | -0.938500 | -0.950608 |
| O ₁₁ | -0.414629 | 2.414599 | -0.459938 | -0.717081 | -1.334609 | -1.246603 |
| H ₁₂ | -1.133239 | 2.789231 | 0.018078 | 0.000000 | 0.389195 | 0.359000 |
| H ₁₃ | 3.345582 | 1.537505 | -0.113718 | 0.000000 | 0.370667 | 0.362441 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|---------|---------|----------|
| 22.1176 | 30.6602 | 34.8146 | 60.6257 | 83.9215 | 128.4090 |
|---------|---------|---------|---------|---------|----------|

$$E(RHF) = -1481.50987106, \Delta E(MP2) = -1.752316663$$

Table 23: $[HPO_4 \cdot Mg \cdot HPO_4]^{2-}$ structure 15

| Atom | X | Y | Z | Mulliken | Chelp1 | Chelp2 |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Mg ₁ | 0.013597 | -0.060698 | -0.048615 | 0.678717 | 1.688151 | 1.546744 |
| P ₂ | 2.601515 | -0.125408 | 0.014620 | 2.554369 | 2.297243 | 2.262298 |
| P ₃ | -2.563626 | 0.003487 | -0.111959 | 2.589814 | 2.409902 | 2.360531 |
| O ₄ | 1.593031 | -0.057024 | 1.184538 | -1.114038 | -1.232426 | -1.176731 |
| O ₅ | -1.565760 | 1.177084 | -0.092434 | -1.098479 | -1.262276 | -1.202555 |
| O ₆ | 1.650685 | -0.078317 | -1.203628 | -1.108750 | -1.261256 | -1.207088 |
| O ₇ | -1.626563 | -1.215032 | -0.085039 | -1.086088 | -1.296258 | -1.238960 |
| O ₈ | 3.379927 | 1.326480 | 0.019218 | -0.587057 | -0.885223 | -0.895121 |
| O ₉ | -3.328822 | 0.030413 | 1.347939 | -0.637603 | -0.870505 | -0.862738 |
| O ₁₀ | 3.662916 | -1.152622 | 0.050225 | -1.077130 | -1.113279 | -1.112850 |
| O ₁₁ | -3.667895 | 0.030453 | -1.109555 | -1.113754 | -1.124979 | -1.123062 |
| H ₁₂ | 2.741416 | 2.020142 | -0.011647 | 0.000000 | 0.347113 | 0.352268 |
| H ₁₃ | -4.253067 | 0.045572 | 1.164989 | 0.000000 | 0.303793 | 0.297264 |

Six lowest frequencies (in cm^{-1})

| | | | | | |
|---------|---------|---------|----------|----------|----------|
| 59.2209 | 60.9420 | 64.0366 | 151.6842 | 179.2065 | 181.5176 |
|---------|---------|---------|----------|----------|----------|

$$E(RHF) = -1482.55871188, \Delta E(MP2) = -1.744799180$$