

Supporting Information

Of

$C(P)_4^{2+}$: A Viable Planar Tetracoordinate Carbon Species

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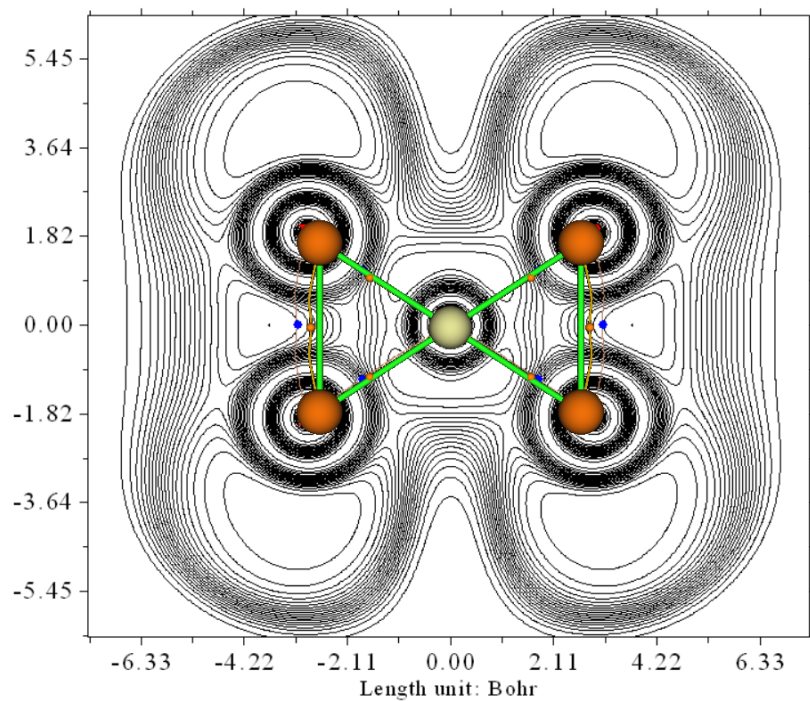


Fig S1. 2D plot of Laplacian of electron density of the D_{2h} structure of $C(P)_4^{2+}$ cluster. Bond critical points are shown in orange dots.

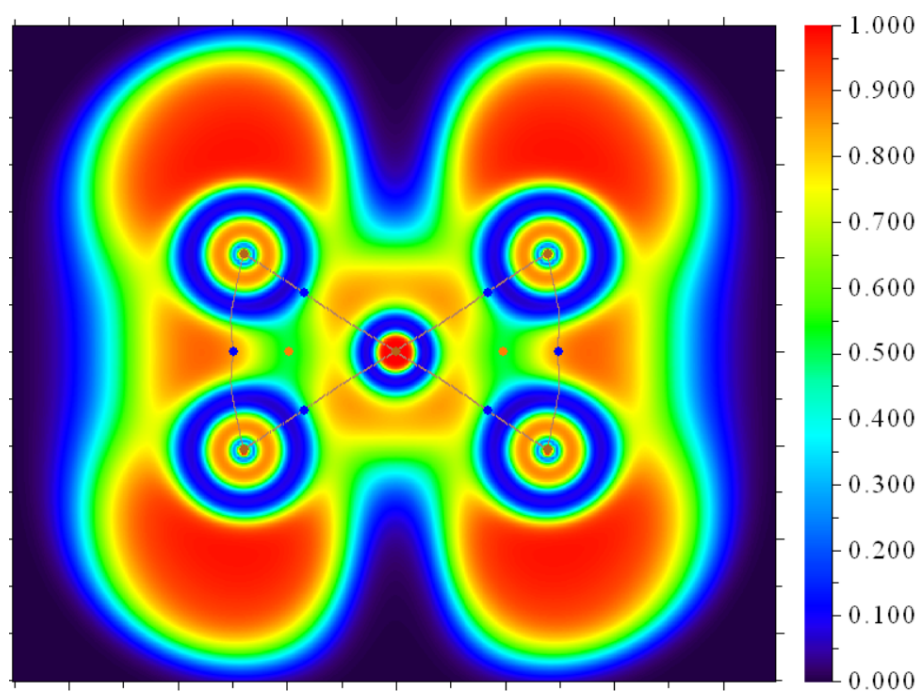


Fig S2. 2D plot of electron localization function.

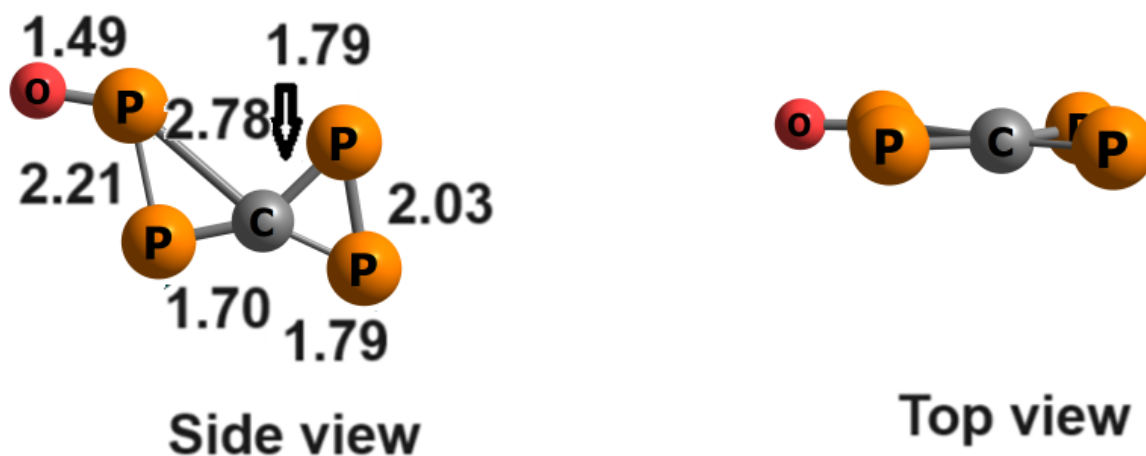


Fig S3. Side and top view of the $C(P_4)^{2+}O^{2-}$ ionic pair. Bond lengths are in Å.

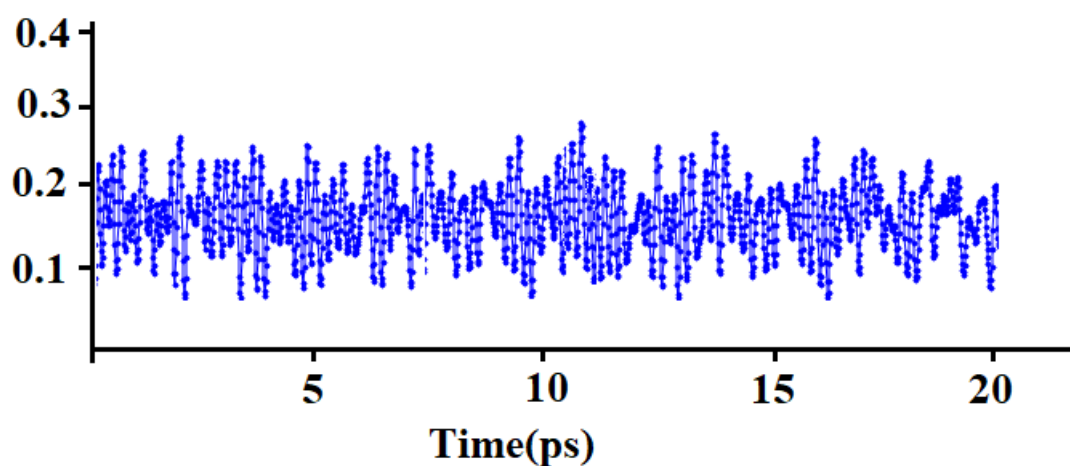


Fig S4. RMSD (Å) versus time (ps) plot of the Born-Oppenheimer molecular dynamics (BOMD) simulation for the ptC structure of $C(P_4)^{2+}O^{2-}$ ionic pair for 20 ps at 298 K with a time frame of 0.5 fs.

Cartesian coordinates of all the molecules along with the total energy, E (a.u) calculated at CCSD(T)/aug-cc-pVTZ//TPSSh/def2-TZVP level. Lowest vibrational frequency is also mentioned.

^{13}C

Lowest vibrational frequency= 238 cm^{-1}

E= -1400.89025

| | | | |
|----|--------------|--------------|--------------|
| 6 | -0.000009000 | -0.000187000 | -1.016227000 |
| 15 | 0.000092000 | -1.105931000 | 0.736015000 |
| 15 | -1.622642000 | -0.000219000 | -0.532533000 |
| 15 | -0.000095000 | 1.106316000 | 0.735540000 |
| 15 | 1.622649000 | -0.000091000 | -0.532531000 |

¹D

Lowest Vibrational Frequency= 60 cm⁻¹

E= -1400.86076

| | | | |
|----|--------------|--------------|--------------|
| 6 | -0.000007000 | 0.000005000 | 0.000005000 |
| 15 | 1.561240000 | 1.009758000 | 0.000144000 |
| 15 | -1.561234000 | -1.009761000 | 0.000144000 |
| 15 | -1.561232000 | 1.009765000 | -0.000145000 |
| 15 | 1.561229000 | -1.009763000 | -0.000145000 |

¹E

Lowest vibrational frequency= 12 cm⁻¹

E= -1400.84554

| | | | |
|----|--------------|--------------|--------------|
| 6 | 0.606021000 | -0.000159000 | 0.002990000 |
| 15 | -3.046869000 | 0.000008000 | -0.006266000 |
| 15 | 1.975668000 | -1.066952000 | -0.002260000 |
| 15 | 1.975335000 | 1.067107000 | -0.002259000 |
| 15 | -1.146543000 | -0.000099000 | 0.009590000 |

¹F

Lowest vibrational frequency= 116 cm⁻¹

E= -1400.84271

| | | | |
|----|--------------|--------------|--------------|
| 6 | -0.919358000 | 0.000732000 | -0.148666000 |
| 15 | 0.461764000 | -1.201563000 | -0.431891000 |

| | | | |
|----|--------------|--------------|--------------|
| 15 | 0.462428000 | 1.201848000 | -0.431488000 |
| 15 | 1.900866000 | -0.000477000 | 0.599336000 |
| 15 | -2.457315000 | -0.000100000 | 0.323509000 |

¹G

Lowest vibrational frequency= 30 cm⁻¹

E= -1400.81904

| | | | |
|----|--------------|--------------|--------------|
| 6 | -1.676610000 | 0.063035000 | -0.051550000 |
| 15 | -3.135158000 | -0.563405000 | -0.113530000 |
| 15 | 1.318618000 | -0.192698000 | 0.693858000 |
| 15 | -0.378205000 | 1.098866000 | -0.091979000 |
| 15 | 2.865389000 | -0.367977000 | -0.467729000 |

³H

Lowest vibrational frequency= 148 cm⁻¹

E= -1400.81439

| | | | |
|----|--------------|--------------|--------------|
| 6 | 0.396197000 | 0.000101000 | 0.239186000 |
| 15 | -2.508805000 | -0.000255000 | -0.711097000 |
| 15 | 1.759009000 | -1.040193000 | -0.188177000 |
| 15 | 1.759098000 | 1.040023000 | -0.188760000 |
| 15 | -1.167781000 | 0.000386000 | 0.992360000 |

³I

Lowest vibrational frequency= 148 cm⁻¹

E= -1400.81034

| | | | |
|----|--------------|--------------|--------------|
| 6 | 0.000158000 | -0.758578000 | -0.000216000 |
| 15 | 1.675986000 | -0.967185000 | -0.186630000 |
| 15 | -1.060839000 | 1.118971000 | -0.294937000 |
| 15 | -1.675611000 | -0.967569000 | 0.186708000 |
| 15 | 1.060400000 | 1.119215000 | 0.294945000 |

³J

Lowest vibrational frequency= 57 cm⁻¹

E= -1400.79688

| | | | |
|----|--------------|--------------|--------------|
| 6 | -0.965538000 | 0.000241000 | 0.034101000 |
| 15 | 0.417366000 | -1.209514000 | -0.055292000 |
| 15 | 0.417476000 | 1.209596000 | -0.055283000 |
| 15 | 2.152469000 | -0.000113000 | 0.065522000 |
| 15 | -2.601095000 | -0.000066000 | 0.031413000 |

TS_{CD}

Lowest vibrational frequency= -228 cm⁻¹

E= -1400.83752

| | | | |
|----|--------------|--------------|--------------|
| 6 | 0.792282000 | 0.000340000 | -0.135354000 |
| 15 | -0.555704000 | 1.182489000 | -0.604253000 |
| 15 | -1.541994000 | -0.000281000 | 0.922909000 |
| 15 | -0.555379000 | -1.182317000 | -0.604584000 |
| 15 | 2.336164000 | -0.000026000 | 0.340069000 |

TS_{DE}

Lowest vibrational frequency= -130 cm⁻¹

E= -1400.83755

| | | | |
|----|--------------|--------------|--------------|
| 6 | -0.305290000 | -0.119393000 | 0.152793000 |
| 15 | 2.072221000 | 0.577723000 | -0.590114000 |
| 15 | -1.547762000 | 1.069721000 | 0.386850000 |
| 15 | -1.741507000 | -0.839481000 | -0.535565000 |
| 15 | 1.339163000 | -0.760205000 | 0.677711000 |

P₄C²⁺O²⁻ ionic pair

Lowest vibrational frequency= 44 cm⁻¹

| | | | |
|----|--------------|--------------|--------------|
| 6 | -0.755474000 | 0.373239000 | -0.000017000 |
| 15 | -2.541770000 | 0.475753000 | -0.000044000 |
| 15 | 1.878199000 | -0.547522000 | -0.000002000 |

| | | | |
|----|--------------|--------------|--------------|
| 15 | 0.668070000 | 1.307489000 | 0.000022000 |
| 15 | -1.480319000 | -1.265915000 | -0.000005000 |
| 8 | 3.333767000 | -0.223313000 | 0.000067000 |