

Supplementary Material

Approximations of density matrices in N-electron valence state second-order perturbation theory (NEVPT2).

II. The full rank NEVPT2 (FR-NEVPT) formulation

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der Ruhr, Germany*

1. Truncated CASCI energies of N₂ using PS approximation with CAS(10,8)/cc-pVQZ.

| N-N bond | $T_{ps}=10^{-10}$ | $T_{ps}=10^{-8}$ | $T_{ps}=10^{-6}$ | $T_{ps}=10^{-4}$ |
|----------|-------------------|------------------|------------------|------------------|
| 2.60 | -108.800990 | -108.800990 | -108.800981 | -108.800346 |
| 2.58 | -108.801046 | -108.801046 | -108.801039 | -108.800325 |
| 2.56 | -108.801110 | -108.801110 | -108.801105 | -108.800385 |
| 2.54 | -108.801182 | -108.801182 | -108.801177 | -108.800413 |
| 2.52 | -108.801264 | -108.801264 | -108.801258 | -108.800447 |
| 2.50 | -108.801356 | -108.801356 | -108.801350 | -108.800478 |
| 2.48 | -108.801461 | -108.801461 | -108.801455 | -108.800538 |
| 2.46 | -108.801580 | -108.801580 | -108.801573 | -108.800670 |
| 2.44 | -108.801715 | -108.801715 | -108.801707 | -108.800774 |
| 2.42 | -108.801868 | -108.801868 | -108.801859 | -108.800839 |
| 2.40 | -108.802043 | -108.802042 | -108.802033 | -108.800978 |
| 2.38 | -108.802241 | -108.802241 | -108.802230 | -108.801246 |
| 2.36 | -108.802466 | -108.802466 | -108.802454 | -108.801401 |
| 2.34 | -108.802723 | -108.802723 | -108.802700 | -108.801538 |
| 2.32 | -108.803014 | -108.803014 | -108.802997 | -108.801781 |
| 2.30 | -108.803346 | -108.803345 | -108.803332 | -108.801826 |
| 2.28 | -108.803722 | -108.803722 | -108.803711 | -108.802331 |
| 2.26 | -108.804150 | -108.804150 | -108.804137 | -108.802931 |
| 2.24 | -108.804636 | -108.804636 | -108.804623 | -108.803352 |
| 2.22 | -108.805187 | -108.805187 | -108.805176 | -108.803965 |
| 2.20 | -108.805812 | -108.805812 | -108.805797 | -108.804496 |
| 2.18 | -108.806519 | -108.806519 | -108.806505 | -108.805105 |
| 2.16 | -108.807319 | -108.807319 | -108.807307 | -108.805796 |
| 2.14 | -108.808223 | -108.808223 | -108.808207 | -108.806581 |
| 2.12 | -108.809243 | -108.809243 | -108.809227 | -108.807473 |
| 2.10 | -108.810393 | -108.810393 | -108.810374 | -108.808465 |
| 2.08 | -108.811685 | -108.811685 | -108.811666 | -108.809621 |
| 2.06 | -108.813136 | -108.813136 | -108.813120 | -108.811030 |
| 2.04 | -108.814762 | -108.814762 | -108.814746 | -108.812488 |
| 2.02 | -108.816579 | -108.816579 | -108.816561 | -108.814306 |
| 2.00 | -108.818605 | -108.818605 | -108.818584 | -108.816453 |
| 1.98 | -108.820858 | -108.820858 | -108.820834 | -108.818542 |
| 1.96 | -108.823355 | -108.823355 | -108.823336 | -108.820865 |
| 1.94 | -108.826117 | -108.826117 | -108.826100 | -108.823601 |
| 1.92 | -108.829158 | -108.829158 | -108.829140 | -108.826637 |
| 1.90 | -108.832498 | -108.832498 | -108.832476 | -108.829894 |
| 1.88 | -108.836151 | -108.836151 | -108.836130 | -108.833400 |
| 1.86 | -108.840132 | -108.840132 | -108.840109 | -108.837234 |
| 1.84 | -108.844453 | -108.844453 | -108.844431 | -108.841408 |
| 1.82 | -108.849124 | -108.849124 | -108.849104 | -108.846994 |
| 1.80 | -108.854153 | -108.854153 | -108.854136 | -108.851981 |
| 1.78 | -108.859547 | -108.859547 | -108.859524 | -108.857160 |

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|------|-------------|-------------|-------------|-------------|
| 1.76 | -108.865308 | -108.865308 | -108.865285 | -108.862906 |
| 1.74 | -108.871438 | -108.871438 | -108.871413 | -108.869029 |
| 1.72 | -108.877936 | -108.877936 | -108.877910 | -108.875068 |
| 1.70 | -108.884798 | -108.884798 | -108.884774 | -108.881960 |
| 1.68 | -108.892020 | -108.892020 | -108.891996 | -108.889220 |
| 1.66 | -108.899594 | -108.899594 | -108.899569 | -108.896840 |
| 1.64 | -108.907512 | -108.907512 | -108.907490 | -108.904811 |
| 1.62 | -108.915764 | -108.915764 | -108.915744 | -108.913123 |
| 1.60 | -108.924338 | -108.924338 | -108.924320 | -108.921761 |
| 1.58 | -108.933221 | -108.933221 | -108.933205 | -108.930714 |
| 1.56 | -108.942399 | -108.942399 | -108.942383 | -108.939964 |
| 1.54 | -108.951853 | -108.951853 | -108.951829 | -108.949495 |
| 1.52 | -108.961565 | -108.961565 | -108.961542 | -108.959285 |
| 1.50 | -108.971514 | -108.971514 | -108.971491 | -108.969315 |
| 1.48 | -108.981674 | -108.981674 | -108.981652 | -108.979557 |
| 1.46 | -108.992018 | -108.992018 | -108.991997 | -108.989596 |
| 1.44 | -109.002514 | -109.002514 | -109.002488 | -108.999832 |
| 1.42 | -109.013126 | -109.013126 | -109.013096 | -109.010553 |
| 1.40 | -109.023814 | -109.023814 | -109.023786 | -109.021350 |
| 1.38 | -109.034531 | -109.034531 | -109.034504 | -109.032176 |
| 1.36 | -109.045224 | -109.045224 | -109.045195 | -109.042977 |
| 1.34 | -109.055832 | -109.055832 | -109.055805 | -109.053184 |
| 1.32 | -109.066287 | -109.066287 | -109.066262 | -109.063762 |
| 1.30 | -109.076512 | -109.076512 | -109.076482 | -109.074109 |
| 1.28 | -109.086417 | -109.086417 | -109.086384 | -109.084135 |
| 1.26 | -109.095904 | -109.095904 | -109.095873 | -109.093740 |
| 1.24 | -109.104859 | -109.104859 | -109.104829 | -109.102415 |
| 1.22 | -109.113156 | -109.113155 | -109.113125 | -109.110880 |
| 1.20 | -109.120649 | -109.120649 | -109.120617 | -109.118335 |
| 1.18 | -109.127179 | -109.127179 | -109.127126 | -109.124534 |
| 1.16 | -109.132561 | -109.132561 | -109.132483 | -109.129518 |
| 1.14 | -109.136592 | -109.136592 | -109.136481 | -109.132888 |
| 1.12 | -109.139040 | -109.139040 | -109.138981 | -109.136476 |
| 1.10 | -109.139646 | -109.139646 | -109.139529 | -109.136201 |
| 1.08 | -109.138117 | -109.138117 | -109.138039 | -109.135135 |
| 1.06 | -109.134126 | -109.134126 | -109.134059 | -109.131626 |
| 1.04 | -109.127304 | -109.127304 | -109.127219 | -109.125000 |
| 1.02 | -109.117236 | -109.117236 | -109.117148 | -109.115110 |
| 1.00 | -109.103455 | -109.103455 | -109.103366 | -109.100237 |
| 0.98 | -109.085435 | -109.085435 | -109.085342 | -109.081846 |
| 0.96 | -109.062584 | -109.062584 | -109.062495 | -109.058915 |
| 0.94 | -109.034237 | -109.034237 | -109.034132 | -109.030794 |
| 0.92 | -108.999642 | -108.999642 | -108.999547 | -108.996412 |
| 0.90 | -108.957952 | -108.957951 | -108.957854 | -108.954919 |
| 0.88 | -108.908211 | -108.908210 | -108.908123 | -108.905364 |

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|------|-------------|-------------|-------------|-------------|
| 0.86 | -108.849341 | -108.849341 | -108.849262 | -108.846666 |
| 0.84 | -108.780124 | -108.780124 | -108.780047 | -108.776382 |
| 0.82 | -108.699183 | -108.699183 | -108.699089 | -108.695710 |
| 0.80 | -108.604962 | -108.604962 | -108.604878 | -108.601736 |

2. Absolute FR-NEVPT2 energies of N₂ using PS approximation with CAS(10,8)/cc-pVQZ,.

| N-N bond | $T_{ps}=10^{-10}$ | $T_{ps}=10^{-8}$ | $T_{ps}=10^{-6}$ | $T_{ps}=10^{-4}$ |
|----------|-------------------|------------------|------------------|------------------|
| 2.60 | -108.800990 | -108.800990 | -108.800981 | -108.800346 |
| 2.58 | -108.801046 | -108.801046 | -108.801039 | -108.800325 |
| 2.56 | -108.801110 | -108.801110 | -108.801105 | -108.800385 |
| 2.54 | -108.801182 | -108.801182 | -108.801177 | -108.800413 |
| 2.52 | -108.801264 | -108.801264 | -108.801258 | -108.800447 |
| 2.50 | -108.801356 | -108.801356 | -108.801350 | -108.800478 |
| 2.48 | -108.801461 | -108.801461 | -108.801455 | -108.800538 |
| 2.46 | -108.801580 | -108.801580 | -108.801573 | -108.800670 |
| 2.44 | -108.801715 | -108.801715 | -108.801707 | -108.800774 |
| 2.42 | -108.801868 | -108.801868 | -108.801859 | -108.800839 |
| 2.40 | -108.802043 | -108.802042 | -108.802033 | -108.800978 |
| 2.38 | -108.802241 | -108.802241 | -108.802230 | -108.801246 |
| 2.36 | -108.802466 | -108.802466 | -108.802454 | -108.801401 |
| 2.34 | -108.802723 | -108.802723 | -108.802700 | -108.801538 |
| 2.32 | -108.803014 | -108.803014 | -108.802997 | -108.801781 |
| 2.30 | -108.803346 | -108.803345 | -108.803332 | -108.801826 |
| 2.28 | -108.803722 | -108.803722 | -108.803711 | -108.802331 |
| 2.26 | -108.804150 | -108.804150 | -108.804137 | -108.802931 |
| 2.24 | -108.804636 | -108.804636 | -108.804623 | -108.803352 |
| 2.22 | -108.805187 | -108.805187 | -108.805176 | -108.803965 |
| 2.20 | -108.805812 | -108.805812 | -108.805797 | -108.804496 |
| 2.18 | -108.806519 | -108.806519 | -108.806505 | -108.805105 |
| 2.16 | -108.807319 | -108.807319 | -108.807307 | -108.805796 |
| 2.14 | -108.808223 | -108.808223 | -108.808207 | -108.806581 |
| 2.12 | -108.809243 | -108.809243 | -108.809227 | -108.807473 |
| 2.10 | -108.810393 | -108.810393 | -108.810374 | -108.808465 |
| 2.08 | -108.811685 | -108.811685 | -108.811666 | -108.809621 |
| 2.06 | -108.813136 | -108.813136 | -108.813120 | -108.811030 |
| 2.04 | -108.814762 | -108.814762 | -108.814746 | -108.812488 |
| 2.02 | -108.816579 | -108.816579 | -108.816561 | -108.814306 |
| 2.00 | -108.818605 | -108.818605 | -108.818584 | -108.816453 |
| 1.98 | -108.820858 | -108.820858 | -108.820834 | -108.818542 |
| 1.96 | -108.823355 | -108.823355 | -108.823336 | -108.820865 |
| 1.94 | -108.826117 | -108.826117 | -108.826100 | -108.823601 |
| 1.92 | -108.829158 | -108.829158 | -108.829140 | -108.826637 |

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|------|-------------|-------------|-------------|-------------|
| 1.90 | -108.832498 | -108.832498 | -108.832476 | -108.829894 |
| 1.88 | -108.836151 | -108.836151 | -108.836130 | -108.833400 |
| 1.86 | -108.840132 | -108.840132 | -108.840109 | -108.837234 |
| 1.84 | -108.844453 | -108.844453 | -108.844431 | -108.841408 |
| 1.82 | -108.849124 | -108.849124 | -108.849104 | -108.846994 |
| 1.80 | -108.854153 | -108.854153 | -108.854136 | -108.851981 |
| 1.78 | -108.859547 | -108.859547 | -108.859524 | -108.857160 |
| 1.76 | -108.865308 | -108.865308 | -108.865285 | -108.862906 |
| 1.74 | -108.871438 | -108.871438 | -108.871413 | -108.869029 |
| 1.72 | -108.877936 | -108.877936 | -108.877910 | -108.875068 |
| 1.70 | -108.884798 | -108.884798 | -108.884774 | -108.881960 |
| 1.68 | -108.892020 | -108.892020 | -108.891996 | -108.889220 |
| 1.66 | -108.899594 | -108.899594 | -108.899569 | -108.896840 |
| 1.64 | -108.907512 | -108.907512 | -108.907490 | -108.904811 |
| 1.62 | -108.915764 | -108.915764 | -108.915744 | -108.913123 |
| 1.60 | -108.924338 | -108.924338 | -108.924320 | -108.921761 |
| 1.58 | -108.933221 | -108.933221 | -108.933205 | -108.930714 |
| 1.56 | -108.942399 | -108.942399 | -108.942383 | -108.939964 |
| 1.54 | -108.951853 | -108.951853 | -108.951829 | -108.949495 |
| 1.52 | -108.961565 | -108.961565 | -108.961542 | -108.959285 |
| 1.50 | -108.971514 | -108.971514 | -108.971491 | -108.969315 |
| 1.48 | -108.981674 | -108.981674 | -108.981652 | -108.979557 |
| 1.46 | -108.992018 | -108.992018 | -108.991997 | -108.989596 |
| 1.44 | -109.002514 | -109.002514 | -109.002488 | -108.999832 |
| 1.42 | -109.013126 | -109.013126 | -109.013096 | -109.010553 |
| 1.40 | -109.023814 | -109.023814 | -109.023786 | -109.021350 |
| 1.38 | -109.034531 | -109.034531 | -109.034504 | -109.032176 |
| 1.36 | -109.045224 | -109.045224 | -109.045195 | -109.042977 |
| 1.34 | -109.055832 | -109.055832 | -109.055805 | -109.053184 |
| 1.32 | -109.066287 | -109.066287 | -109.066262 | -109.063762 |
| 1.30 | -109.076512 | -109.076512 | -109.076482 | -109.074109 |
| 1.28 | -109.086417 | -109.086417 | -109.086384 | -109.084135 |
| 1.26 | -109.095904 | -109.095904 | -109.095873 | -109.093740 |
| 1.24 | -109.104859 | -109.104859 | -109.104829 | -109.102415 |
| 1.22 | -109.113156 | -109.113155 | -109.113125 | -109.110880 |
| 1.20 | -109.120649 | -109.120649 | -109.120617 | -109.118335 |
| 1.18 | -109.127179 | -109.127179 | -109.127126 | -109.124534 |
| 1.16 | -109.132561 | -109.132561 | -109.132483 | -109.129518 |
| 1.14 | -109.136592 | -109.136592 | -109.136481 | -109.132888 |
| 1.12 | -109.139040 | -109.139040 | -109.138981 | -109.136476 |
| 1.10 | -109.139646 | -109.139646 | -109.139529 | -109.136201 |
| 1.08 | -109.138117 | -109.138117 | -109.138039 | -109.135135 |
| 1.06 | -109.134126 | -109.134126 | -109.134059 | -109.131626 |
| 1.04 | -109.127304 | -109.127304 | -109.127219 | -109.125000 |
| 1.02 | -109.117236 | -109.117236 | -109.117148 | -109.115110 |

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|------|-------------|-------------|-------------|-------------|
| 1.00 | -109.103455 | -109.103455 | -109.103366 | -109.100237 |
| 0.98 | -109.085435 | -109.085435 | -109.085342 | -109.081846 |
| 0.96 | -109.062584 | -109.062584 | -109.062495 | -109.058915 |
| 0.94 | -109.034237 | -109.034237 | -109.034132 | -109.030794 |
| 0.92 | -108.999642 | -108.999642 | -108.999547 | -108.996412 |
| 0.90 | -108.957952 | -108.957951 | -108.957854 | -108.954919 |
| 0.88 | -108.908211 | -108.908210 | -108.908123 | -108.905364 |
| 0.86 | -108.849341 | -108.849341 | -108.849262 | -108.846666 |
| 0.84 | -108.780124 | -108.780124 | -108.780047 | -108.776382 |
| 0.82 | -108.699183 | -108.699183 | -108.699089 | -108.695710 |
| 0.80 | -108.604962 | -108.604962 | -108.604878 | -108.601736 |

3. Truncated CASCI energies of O₂ using PS approximation with CAS(12,8)/cc-pVQZ.

| O-O bond | $T_{ps}=10^{-10}$ | $T_{ps}=10^{-8}$ | $T_{ps}=10^{-6}$ | $T_{ps}=10^{-4}$ |
|----------|-------------------|------------------|------------------|------------------|
| 2.60 | -149.617341 | -149.617341 | -149.617339 | -149.617150 |
| 2.58 | -149.617316 | -149.617316 | -149.617314 | -149.617111 |
| 2.56 | -149.617291 | -149.617291 | -149.617287 | -149.617070 |
| 2.54 | -149.617265 | -149.617265 | -149.617262 | -149.617029 |
| 2.52 | -149.617239 | -149.617239 | -149.617239 | -149.616985 |
| 2.50 | -149.617214 | -149.617214 | -149.617214 | -149.616863 |
| 2.48 | -149.617189 | -149.617189 | -149.617189 | -149.616864 |
| 2.46 | -149.617166 | -149.617166 | -149.617166 | -149.616813 |
| 2.44 | -149.617146 | -149.617146 | -149.617145 | -149.616803 |
| 2.42 | -149.617128 | -149.617128 | -149.617127 | -149.616758 |
| 2.40 | -149.617115 | -149.617115 | -149.617115 | -149.616649 |
| 2.38 | -149.617108 | -149.617108 | -149.617108 | -149.616674 |
| 2.36 | -149.617109 | -149.617109 | -149.617109 | -149.616598 |
| 2.34 | -149.617120 | -149.617120 | -149.617119 | -149.616757 |
| 2.32 | -149.617142 | -149.617142 | -149.617142 | -149.616747 |
| 2.30 | -149.617180 | -149.617180 | -149.617180 | -149.616843 |
| 2.28 | -149.617237 | -149.617237 | -149.617237 | -149.616875 |
| 2.26 | -149.617317 | -149.617317 | -149.617314 | -149.616932 |
| 2.24 | -149.617425 | -149.617425 | -149.617425 | -149.616967 |
| 2.22 | -149.617567 | -149.617567 | -149.617560 | -149.617111 |
| 2.20 | -149.617750 | -149.617750 | -149.617749 | -149.617267 |
| 2.18 | -149.617980 | -149.617980 | -149.617979 | -149.617510 |
| 2.16 | -149.618268 | -149.618268 | -149.618268 | -149.617743 |
| 2.14 | -149.618623 | -149.618623 | -149.618621 | -149.618059 |
| 2.12 | -149.619055 | -149.619055 | -149.619048 | -149.618438 |
| 2.10 | -149.619577 | -149.619577 | -149.619576 | -149.618900 |
| 2.08 | -149.620202 | -149.620202 | -149.620201 | -149.619459 |
| 2.06 | -149.620942 | -149.620942 | -149.620939 | -149.620272 |
| 2.04 | -149.621812 | -149.621812 | -149.621811 | -149.621084 |

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|------|-------------|-------------|-------------|-------------|
| 2.02 | -149.622825 | -149.622825 | -149.622820 | -149.622036 |
| 2.00 | -149.623995 | -149.623995 | -149.623993 | -149.623111 |
| 1.98 | -149.625335 | -149.625335 | -149.625334 | -149.624416 |
| 1.96 | -149.626857 | -149.626857 | -149.626855 | -149.625764 |
| 1.94 | -149.628570 | -149.628570 | -149.628567 | -149.627634 |
| 1.92 | -149.630483 | -149.630483 | -149.630482 | -149.630330 |
| 1.90 | -149.632603 | -149.632603 | -149.632601 | -149.632452 |
| 1.88 | -149.634934 | -149.634934 | -149.634932 | -149.634703 |
| 1.86 | -149.637479 | -149.637479 | -149.637478 | -149.637190 |
| 1.84 | -149.640240 | -149.640240 | -149.640238 | -149.640022 |
| 1.82 | -149.643215 | -149.643215 | -149.643214 | -149.642958 |
| 1.80 | -149.646403 | -149.646403 | -149.646402 | -149.646149 |
| 1.78 | -149.649800 | -149.649800 | -149.649799 | -149.649519 |
| 1.76 | -149.653401 | -149.653401 | -149.653398 | -149.653158 |
| 1.74 | -149.657201 | -149.657201 | -149.657199 | -149.656866 |
| 1.72 | -149.661192 | -149.661192 | -149.661191 | -149.659552 |
| 1.70 | -149.665366 | -149.665366 | -149.665365 | -149.664831 |
| 1.68 | -149.669715 | -149.669715 | -149.669714 | -149.669178 |
| 1.66 | -149.674227 | -149.674227 | -149.674226 | -149.673797 |
| 1.64 | -149.678892 | -149.678892 | -149.678890 | -149.678438 |
| 1.62 | -149.683697 | -149.683697 | -149.683695 | -149.683193 |
| 1.60 | -149.688627 | -149.688627 | -149.688624 | -149.688236 |
| 1.58 | -149.693668 | -149.693668 | -149.693665 | -149.693267 |
| 1.56 | -149.698802 | -149.698802 | -149.698799 | -149.698199 |
| 1.54 | -149.704009 | -149.704009 | -149.704006 | -149.703440 |
| 1.52 | -149.709269 | -149.709269 | -149.709268 | -149.707902 |
| 1.50 | -149.714558 | -149.714558 | -149.714556 | -149.712774 |
| 1.48 | -149.719849 | -149.719849 | -149.719847 | -149.718798 |
| 1.46 | -149.725112 | -149.725112 | -149.725111 | -149.724809 |
| 1.44 | -149.730315 | -149.730315 | -149.730314 | -149.728754 |
| 1.42 | -149.735421 | -149.735421 | -149.735419 | -149.733889 |
| 1.40 | -149.740387 | -149.740387 | -149.740386 | -149.739725 |
| 1.38 | -149.745168 | -149.745168 | -149.745166 | -149.744533 |
| 1.36 | -149.749710 | -149.749710 | -149.749709 | -149.748283 |
| 1.34 | -149.753954 | -149.753954 | -149.753947 | -149.752824 |
| 1.32 | -149.757834 | -149.757834 | -149.757830 | -149.756894 |
| 1.30 | -149.761273 | -149.761273 | -149.761270 | -149.760359 |
| 1.28 | -149.764186 | -149.764186 | -149.764183 | -149.763353 |
| 1.26 | -149.766474 | -149.766474 | -149.766472 | -149.765698 |
| 1.24 | -149.768028 | -149.768028 | -149.768022 | -149.767149 |
| 1.22 | -149.768723 | -149.768723 | -149.768722 | -149.767936 |
| 1.20 | -149.768416 | -149.768416 | -149.768415 | -149.767771 |
| 1.18 | -149.766946 | -149.766946 | -149.766944 | -149.766380 |
| 1.16 | -149.764131 | -149.764131 | -149.764127 | -149.763390 |
| 1.14 | -149.759763 | -149.759763 | -149.759762 | -149.758862 |

| | | | | |
|------|-------------|-------------|-------------|-------------|
| 1.12 | -149.753607 | -149.753607 | -149.753601 | -149.752883 |
| 1.10 | -149.745399 | -149.745399 | -149.745398 | -149.744209 |
| 1.08 | -149.734836 | -149.734836 | -149.734835 | -149.734094 |
| 1.06 | -149.721579 | -149.721579 | -149.721578 | -149.720464 |
| 1.04 | -149.705244 | -149.705244 | -149.705238 | -149.704166 |
| 1.02 | -149.685396 | -149.685396 | -149.685391 | -149.683901 |
| 1.00 | -149.661545 | -149.661545 | -149.661534 | -149.660581 |
| 0.98 | -149.633135 | -149.633135 | -149.633122 | -149.631762 |
| 0.96 | -149.599541 | -149.599541 | -149.599522 | -149.598226 |
| 0.94 | -149.560054 | -149.560054 | -149.560045 | -149.558563 |
| 0.92 | -149.513874 | -149.513874 | -149.513859 | -149.512263 |
| 0.90 | -149.460095 | -149.460095 | -149.460086 | -149.458109 |
| 0.88 | -149.397690 | -149.397690 | -149.397671 | -149.395008 |
| 0.86 | -149.325497 | -149.325497 | -149.325481 | -149.322963 |
| 0.84 | -149.242198 | -149.242198 | -149.242184 | -149.239800 |
| 0.82 | -149.146296 | -149.146296 | -149.146283 | -149.144024 |
| 0.80 | -149.036087 | -149.036087 | -149.036077 | -149.033934 |

4. Absolute FR-NEVPT2 energies of O₂ using PS approximation with CAS(12,8)/cc-pVQZ.

| O-O bond | $T_{ps}=10^{-10}$ | $T_{ps}=10^{-8}$ | $T_{ps}=10^{-6}$ | $T_{ps}=10^{-4}$ |
|----------|-------------------|------------------|------------------|------------------|
| 2.60 | -149.985739 | -149.985739 | -149.985729 | -149.985477 |
| 2.58 | -149.985811 | -149.985811 | -149.985800 | -149.985528 |
| 2.56 | -149.985890 | -149.985890 | -149.985877 | -149.985585 |
| 2.54 | -149.985976 | -149.985976 | -149.985964 | -149.985648 |
| 2.52 | -149.986072 | -149.986072 | -149.986071 | -149.985717 |
| 2.50 | -149.986178 | -149.986178 | -149.986177 | -149.985742 |
| 2.48 | -149.986296 | -149.986296 | -149.986295 | -149.985861 |
| 2.46 | -149.986427 | -149.986427 | -149.986426 | -149.985955 |
| 2.44 | -149.986574 | -149.986574 | -149.986573 | -149.986089 |
| 2.42 | -149.986739 | -149.986739 | -149.986737 | -149.986213 |
| 2.40 | -149.986925 | -149.986925 | -149.986923 | -149.986309 |
| 2.38 | -149.987135 | -149.987135 | -149.987132 | -149.986513 |
| 2.36 | -149.987372 | -149.987372 | -149.987369 | -149.986668 |
| 2.34 | -149.987640 | -149.987640 | -149.987638 | -149.987109 |
| 2.32 | -149.987946 | -149.987946 | -149.987943 | -149.987365 |
| 2.30 | -149.988293 | -149.988293 | -149.988291 | -149.987859 |
| 2.28 | -149.988689 | -149.988689 | -149.988687 | -149.988220 |
| 2.26 | -149.989141 | -149.989141 | -149.989136 | -149.988636 |
| 2.24 | -149.989658 | -149.989658 | -149.989655 | -149.989084 |
| 2.22 | -149.990247 | -149.990247 | -149.990240 | -149.989648 |
| 2.20 | -149.990921 | -149.990921 | -149.990919 | -149.990330 |
| 2.18 | -149.991690 | -149.991690 | -149.991688 | -149.991079 |
| 2.16 | -149.992567 | -149.992567 | -149.992565 | -149.991893 |

| | | | | |
|------|-------------|-------------|-------------|-------------|
| 2.14 | -149.993565 | -149.993565 | -149.993562 | -149.992835 |
| 2.12 | -149.994699 | -149.994699 | -149.994691 | -149.993900 |
| 2.10 | -149.995981 | -149.995981 | -149.995978 | -149.995109 |
| 2.08 | -149.997427 | -149.997427 | -149.997425 | -149.996477 |
| 2.06 | -149.999051 | -149.999051 | -149.999047 | -149.998278 |
| 2.04 | -150.000865 | -150.000865 | -150.000863 | -150.000033 |
| 2.02 | -150.002881 | -150.002881 | -150.002862 | -150.001988 |
| 2.00 | -150.005108 | -150.005108 | -150.005093 | -150.004138 |
| 1.98 | -150.007554 | -150.007554 | -150.007541 | -150.006539 |
| 1.96 | -150.010225 | -150.010225 | -150.010212 | -150.009097 |
| 1.94 | -150.013123 | -150.013123 | -150.013110 | -150.012096 |
| 1.92 | -150.016248 | -150.016248 | -150.016239 | -150.016089 |
| 1.90 | -150.019600 | -150.019600 | -150.019592 | -150.019444 |
| 1.88 | -150.023176 | -150.023176 | -150.023168 | -150.022979 |
| 1.86 | -150.026970 | -150.026970 | -150.026963 | -150.026721 |
| 1.84 | -150.030977 | -150.030977 | -150.030972 | -150.030769 |
| 1.82 | -150.035190 | -150.035190 | -150.035186 | -150.034962 |
| 1.80 | -150.039601 | -150.039601 | -150.039598 | -150.039378 |
| 1.78 | -150.044203 | -150.044203 | -150.044200 | -150.043967 |
| 1.76 | -150.048985 | -150.048985 | -150.048981 | -150.048774 |
| 1.74 | -150.053939 | -150.053939 | -150.053936 | -150.053676 |
| 1.72 | -150.059054 | -150.059054 | -150.059054 | -150.057644 |
| 1.70 | -150.064321 | -150.064321 | -150.064320 | -150.063882 |
| 1.68 | -150.069728 | -150.069728 | -150.069727 | -150.069299 |
| 1.66 | -150.075263 | -150.075263 | -150.075262 | -150.074934 |
| 1.64 | -150.080914 | -150.080914 | -150.080912 | -150.080576 |
| 1.62 | -150.086667 | -150.086667 | -150.086665 | -150.086301 |
| 1.60 | -150.092509 | -150.092509 | -150.092506 | -150.092245 |
| 1.58 | -150.098423 | -150.098423 | -150.098419 | -150.098159 |
| 1.56 | -150.104393 | -150.104393 | -150.104388 | -150.103990 |
| 1.54 | -150.110400 | -150.110400 | -150.110394 | -150.110033 |
| 1.52 | -150.116424 | -150.116424 | -150.116434 | -150.115518 |
| 1.50 | -150.122442 | -150.122442 | -150.122452 | -150.121295 |
| 1.48 | -150.128429 | -150.128429 | -150.128439 | -150.127883 |
| 1.46 | -150.134359 | -150.134359 | -150.134368 | -150.134325 |
| 1.44 | -150.140200 | -150.140200 | -150.140208 | -150.139118 |
| 1.42 | -150.145917 | -150.145917 | -150.145924 | -150.144876 |
| 1.40 | -150.151472 | -150.151472 | -150.151478 | -150.151077 |
| 1.38 | -150.156820 | -150.156820 | -150.156825 | -150.156449 |
| 1.36 | -150.161913 | -150.161913 | -150.161917 | -150.160990 |
| 1.34 | -150.166693 | -150.166693 | -150.166695 | -150.166111 |
| 1.32 | -150.171096 | -150.171096 | -150.171100 | -150.170654 |
| 1.30 | -150.175051 | -150.175051 | -150.175053 | -150.174638 |
| 1.28 | -150.178474 | -150.178474 | -150.178476 | -150.178123 |
| 1.26 | -150.181270 | -150.181270 | -150.181271 | -150.180957 |

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|------|-------------|-------------|-------------|-------------|
| 1.24 | -150.183331 | -150.183331 | -150.183328 | -150.182963 |
| 1.22 | -150.184535 | -150.184535 | -150.184535 | -150.184178 |
| 1.20 | -150.184742 | -150.184742 | -150.184741 | -150.184502 |
| 1.18 | -150.183791 | -150.183791 | -150.183789 | -150.183618 |
| 1.16 | -150.181501 | -150.181502 | -150.181499 | -150.181217 |
| 1.14 | -150.177666 | -150.177667 | -150.177664 | -150.177375 |
| 1.12 | -150.172052 | -150.172052 | -150.172047 | -150.171903 |
| 1.10 | -150.164391 | -150.164391 | -150.164388 | -150.163722 |
| 1.08 | -150.154383 | -150.154383 | -150.154380 | -150.154138 |
| 1.06 | -150.141688 | -150.141688 | -150.141685 | -150.141017 |
| 1.04 | -150.125920 | -150.125920 | -150.125912 | -150.125247 |
| 1.02 | -150.106643 | -150.106643 | -150.106635 | -150.105374 |
| 1.00 | -150.083365 | -150.083365 | -150.083357 | -150.082617 |
| 0.98 | -150.055532 | -150.055531 | -150.055524 | -150.054322 |
| 0.96 | -150.022515 | -150.022514 | -150.022501 | -150.021336 |
| 0.94 | -149.983605 | -149.983605 | -149.983595 | -149.982885 |
| 0.92 | -149.938002 | -149.938001 | -149.937993 | -149.936880 |
| 0.90 | -149.884798 | -149.884798 | -149.884788 | -149.883097 |
| 0.88 | -149.822967 | -149.822967 | -149.822959 | -149.820407 |
| 0.86 | -149.751344 | -149.751344 | -149.751339 | -149.748871 |
| 0.84 | -149.668610 | -149.668610 | -149.668606 | -149.666221 |
| 0.82 | -149.573263 | -149.573263 | -149.573259 | -149.570957 |
| 0.80 | -149.463592 | -149.463592 | -149.463590 | -149.461369 |
