SUPPORTING INFORMATION

Pt^X as the limit of high oxidation states in oxide-nitride species

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This work commemorates the 100th anniversary of the Polish Chemical Society.

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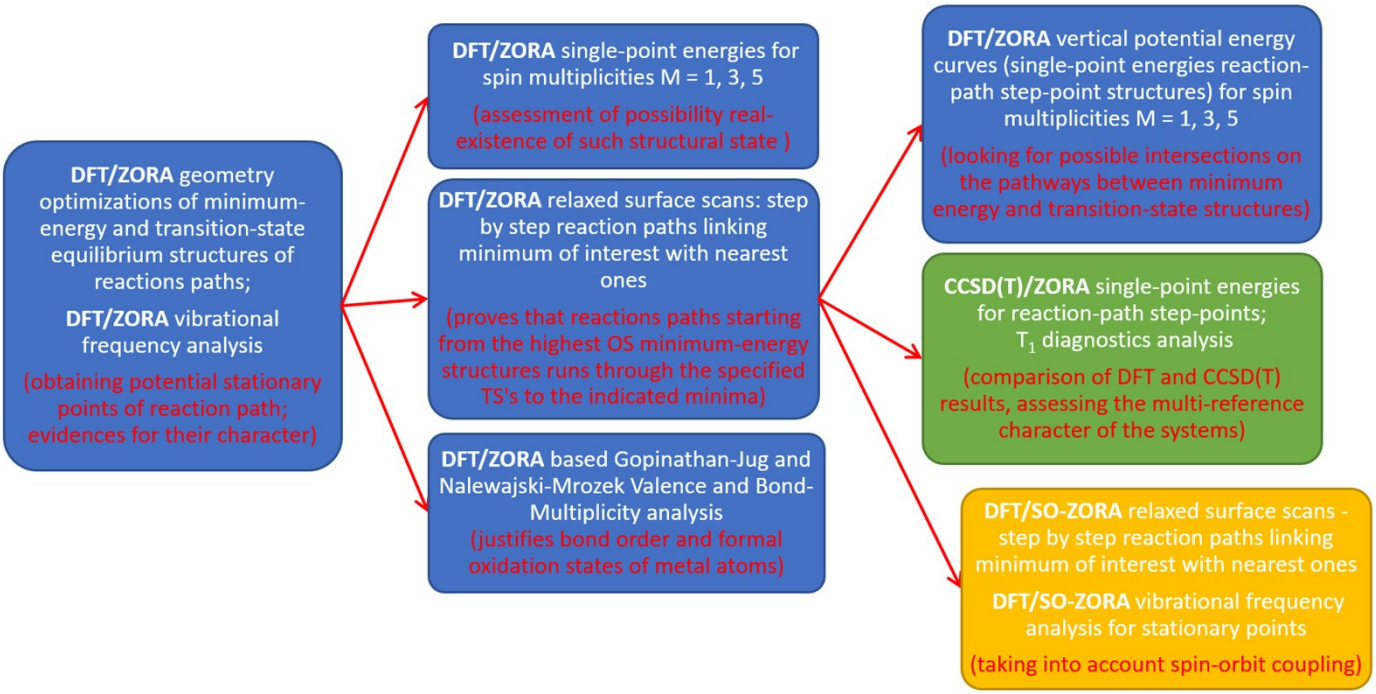
Abbreviations

CCSD(T) - Coupled Cluster single-double and perturbative correction of triples
PES - Potential Energy Surface (Curve)
SO-ZORA - zeroth-order regular approximation relativistic Hamiltonian with relativistic spin-orbit coupling
SO - spin-orbit
TS - transition state
ZORA - zeroth-order regular approximation **scalar** relativistic Hamiltonian

Additional information



Scheme S1. The computational scheme that was used in this paper. Justification of performing each component of all calculations is marked in red.

The main goal of our theoretical investigations was to evaluate whether the model chemical compounds with given stoichiometry may consist the metal atoms at very high formal oxidation state – corresponding to $5d^0$ electron configuration (**Figure 1**). Our computational approach is briefly summarized in **Scheme S1**. Majority of the computations were performed at the DFT/scalar-

ZORA[1] level of theory **as preliminary step**. We are fully aware that this methodology may be sometimes insufficient for investigated systems (especially based on platinum and heavier atoms), yet it is sufficient for qualitative assessment of their relative stability. For the most encouraging cases the more accurate DFT/SO-ZORA approach has been employed.

Research concept in details

Heavy transition metals do not prefer open d-shell electronic structure and low spin forms are predominantly preferred. Nevertheless, distinct spin multiplicities (M=1, 3, 5) were considered while determining the equilibrium structures of potential isomers including atoms at very high oxidation states. All reasonable and important structures in our investigations (corresponding to stationary points on PES) were determined to adapt a singlet multiplicity. Whenever the existence of a (meta-)stable structure was predicted by calculations reaction(s) of dissociation of: O_2, NO or N_2, , were analysed depending on the investigated molecule. Respectively other equilibrium structures constituting energy minima and transition states were researched to find the main points of the reaction path. All considered stationary point structures were calculated by full relaxing of geometrical parameters (**Figures S1-S3, Appendix S1**). The obtained equilibrium geometries corresponding to real energy minima or transition states (TS) were confirmed by vibrational frequency analysis.

Vertical single point energies of higher multiplicity states (M=3, 5) were obtained with respect to singlet geometries (vertical energies) to verify possible protecting barriers lowering due to crossing between different spin states reaction path PESs (**Figures S4-S6**).

Additionally, whenever it was possible the surrounding of stationary points on PES was investigated. Thus, we performed series of constrained geometry optimizations between determined stationary point structures. Step-by-step reaction path was established by geometry optimization with one fixed interatomic distance (between atoms of dissociating diatomic molecule), which corresponds to the intrinsic reaction coordinate. This procedure is so-called relaxed surface scan, thanks to it we obtained entire reaction paths (**Figures S7-S23** - red points, **Tables S1-S17**).

Resolved structures from relaxed surface scans (M=1) (see **Appendix 2**) were used to calculate vertical (single-point) energies for higher multiplicities (M=3, 5) (**Figures S7-S23** - green and blue points, **Tables S1-S17**). In proximity of TSs structures higher-multiplicity PESs crossing the singlet-multiplicity PES, were observed, lowering the energetic barrier heights.

Therefore, higher-level computational treatment of spin configuration has been employed in order to justify these preliminary results. Firstly, relativistic spin-orbit (SO) coupling effects were considered. Secondly, spin-unrestricted approach was utilized together with non-collinear approximation, removing additional spin constraints – both described in details in next sections. This method was used to re-calculate reaction paths (for respective structures see **Appendix 3,** for energetic profiles see **Figures 4, S19-S35** and **Tables S19-S35**).

[1] Later, in this SI, *scalar-ZORA* will be referred to simply as *ZORA*

PtO_4^{2+} as a reference structure

The appropriateness of DFT/ZORA for similar purposes has been previously demonstrated[1]. However, it is important to discuss if our approach is applicable to other metals, especially platinum. The Schwartz, Li and coworkers had computationally predicted the energetic stability of isolated PtO_4^{2+} dication with *state-of-the-art* multireference perturbation theory methodology. Comparison of our results for this specie (**Figures S16, S34** and **Tables S10, S27**) with data from Figure 2 and Table S1 of their work shows good consistency.

Computational Details (Expanded version)

Because available in the literature theoretical results for the highest oxidation states of 5d transitional metals come from different computational approaches[2–5], in our previous studies[1], we had investigated the equilibrium geometries with three different Kohn-Sham density functional theory (DFT) functionals, which in fact led to very similar results. Hence, in this investigation, we decided to employ only the meta-generalized gradient approximation exchange-correlation fully local M06-L[6], which has been well validated for transition-metals[7]. In some difficult cases, in which we were unable to finish the calculations because of numerical problems, a hybrid functional B3LYP[8–10], which is excellent for the redox thermochemistry of transition-metal systems in high oxidation states[2] and has good performance for comparable molecules[11], was used (**Appendix S1**). According to our experience, results obtained from both approaches are very comparable.

Since relativistic effects stabilize high oxidation states[12], respective corrections were included in all calculations by using the zeroth-order regular approximation scalar relativistic Hamiltonian (ZORA)[13–15]. Because metal atoms, required basis sets that are small, loosely contracted and involving the core electrons the segmented scalar relativistic all-electron basis sets were applied, which provide a balanced description of core and valence electron densities: SARC-ZORA-TZVPP[16]. For nitrogen and oxygen atoms ZORA-def2-TZVPP[17] basis set was used. All geometry optimization using DFT/ZORA approach were done with Orca 4.0.1 package[18–20]. The largest angular grid (Grid7) has been used, what is required in calculations with ZORA relativistic correction for systems containing heavier atoms. The frozen-core and RI approximations were not used at all. In contrast to single-point energy calculations, during all geometry optimization calculations one-center relativistic approximation, which impact on geometries is negligible, was utilized. All DFT energy values presented in this work were obtained without using this approximation.

For all reaction paths obtained with DFT/ZORA spin-restricted approach, single-point energies at the Coupled Cluster single-double and perturbative correction of triples (CCSD(T))[21–23] were obtained (**Figures S7-S23, Tables S1-S17**) with the same basis sets and relativistic Hamiltonian, as used during geometry optimization. T_1 diagnostic values were also obtained (**Figures S7-S23, Tables S1-S17**), what is important for assessing the adequacy of using this computational method. High value of T_1 diagnostic usually implies, that single reference method may not give reliable predictions of energetic and spectroscopic parameters and it is necessary to employ multireference wave function-based methods. It is quite common to use as the limit value 0.02, which has been established based on the study of 23 main group species[24,25]. However for molecules containing 3d transition-metals- $T_1 > 0.05$ has been suggested to identify

inorganic species with substantial nondynamical correlation.[26] Similarly, for 4d ones T_1 diagnostic limit value is 0.045.[27] In our case, for almost all molecular structures composing reaction paths, T_1 parameter values do not exceed the limit value determined for mentioned d-electron elements. Of course, in our investigations, this value is sometimes exceeding 0.045, mainly at the TS points and in their proximity. However, less credibility of the CCSD(T) results at these points does not change the fact, that the points slightly further away from the TSs usually have smaller, acceptable values of T_1 (**Figures S10C, S11C, S15C, S16C, S19C and S21C**). It allows to assume the existence of a certain barrier and even to estimate its height. Only in one case of a Pt compound the energies of subsequent structures on the reaction path between minimum A and transition state B' cannot be correctly described by the CCSD(T) method due to the probably very large multireference character indicated by high values of the T_1 diagnostic parameter. Here we have to mention, that sometimes relatively high T_1 diagnostic parameter values are not due to 'multi-reference' character of the wave function, but rather a problem of spin contamination.[28] Despite this limitations, the methodology basing on DFT optimizations followed by CCSD(T) single-point energy calculations is well established as a reliable tool for 5d transition metal (Ir, Pt, Au, Hg) systems investigations.[3,11,29–32] All mentioned single-point energy DFT and CCSD(T) calculations were performed with Orca 4.0.1 package[18–20].

Although Riedel and co-workers were shown[3] that spin–orbit (SO) coupling shows only minor effects on the stability of the rhodium and iridium tetroxide complexes, in order to investigate in detail the occurrence of spin-crossing, especially for platinum compounds, we performed relaxed surface scans (**Appendix S3**) with relativistic SO coupling effects taken into account[14,33]. In this method we used also spin-unrestricted approach together with noncollinear approximation of spin polarization[34]. This means that the spin-polarization can have other than (anti)parallel direction and Kramer's symmetry does not have to be satisfied. Both mentioned methods were used as implemented in ADF 2019[35–37] computational package. All structures were optimized at the DFT(M06-L)/SO-ZORA of theory with Slater type TZ2P all electron basis set[38] (optimized for the use with ZORA) and without frozen-core approximation. Observed differences between (quasi-)tetrahedral equilibrium geometries obtained from calculations in Orca and ADF are irrelevant in the context of the investigated properties, and will not be further discussed.

In the final step, we decided to perform Gopinathan-Jug[39] and Nalewajski-Mrozek Valence and Bond-Multiplicity bond order analysis[40–47] for some minimum energy structures set (**Table S37**) in ADF 2019[35–37]. Discussed in this paper N-M(1) bond orders (markings according to the ADF – what is equivalent of the set2 from Ref. [47]) are calculated from two-electron valence indices based on partitioning of tr(ΔP2] (3-index set).

Structure labelling

For all studied systems, the isomer containing metal with a formal electronic configuration $5d^0$ was labelled as **A**. The next stationary points on the decomposition path were marked as follows: in the case of dissociation of oxygen molecules are labelled with consecutive letters (**B**, **C**, **D**, **E**), for nitric monoxide dissociation structures are marked with letters and the prime sign (**B'**, **C'**, **D'**, **E'**), and in the case of dissociation of a nitrogen molecule with the double prime sign (**B"**, **C"**, **D"**, **E"**).

Note!

By "singlet" we mean singlet state wherever we discussed plain DFT calculations. We did not perform any spin-restricted SO calculations. In our unrestricted SO calculation method, the Kramer's symmetry does not have to be satisfied.

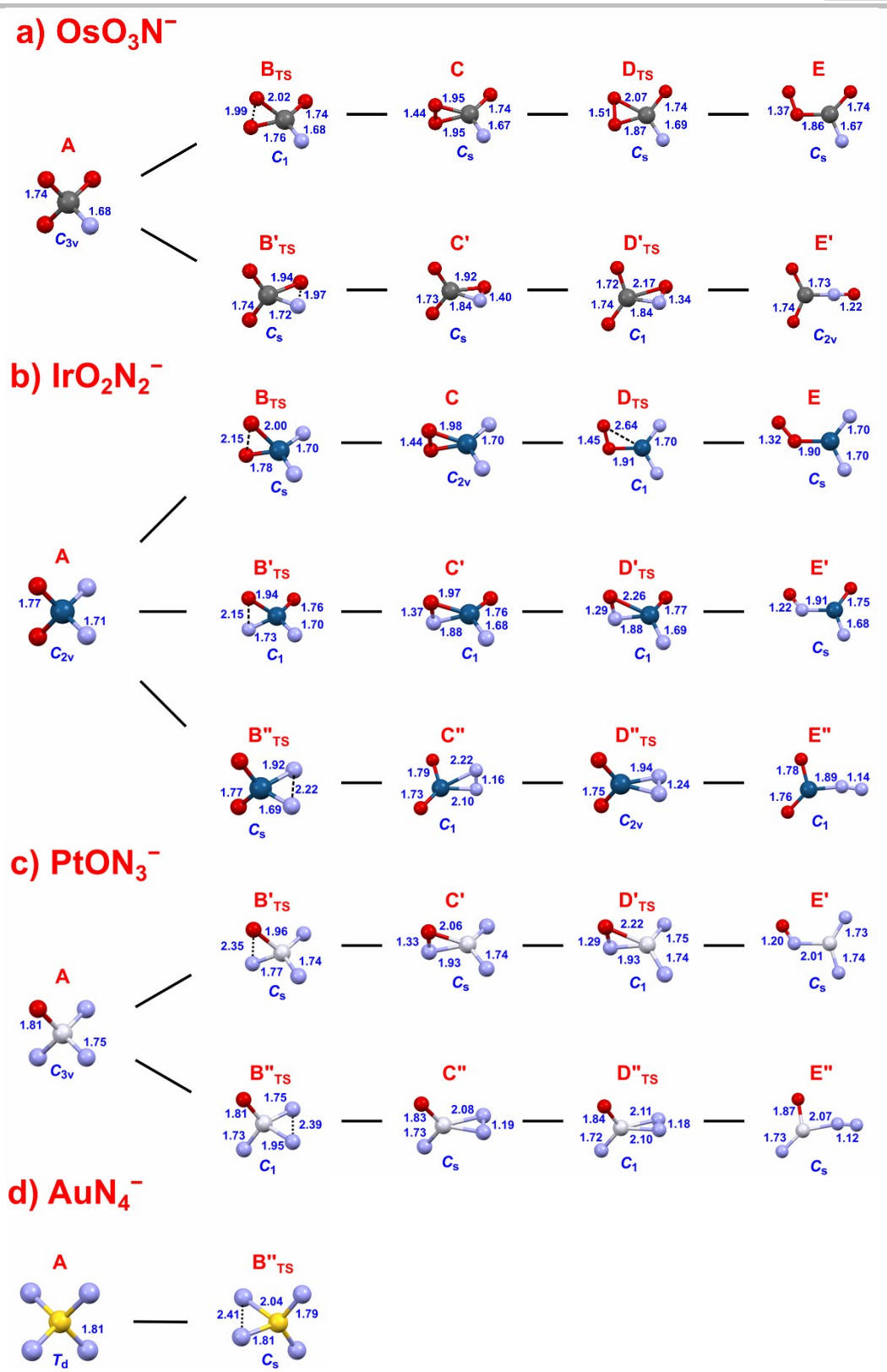


Figure S1. Equilibrium structures corresponding to stationary points constituting reaction paths of dissociation of their diatomic ligands (O_2, NO or N_2) from isomers containing metal atoms at the highest formal oxidation step (**A**) - **anionic molecules.** Molecular symmetry and chosen interatomic distances [Å] are shown. Isomers labelling was described in *Additional explanations/Structure labelling* section of this *Supporting Information*. Molecular structures were obtained from the DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (For each structure computational method is indicated in detail in *Appendix S1*). If there is a lack of structure on the figure, we were unable to optimize some of the structures with any of these methods.

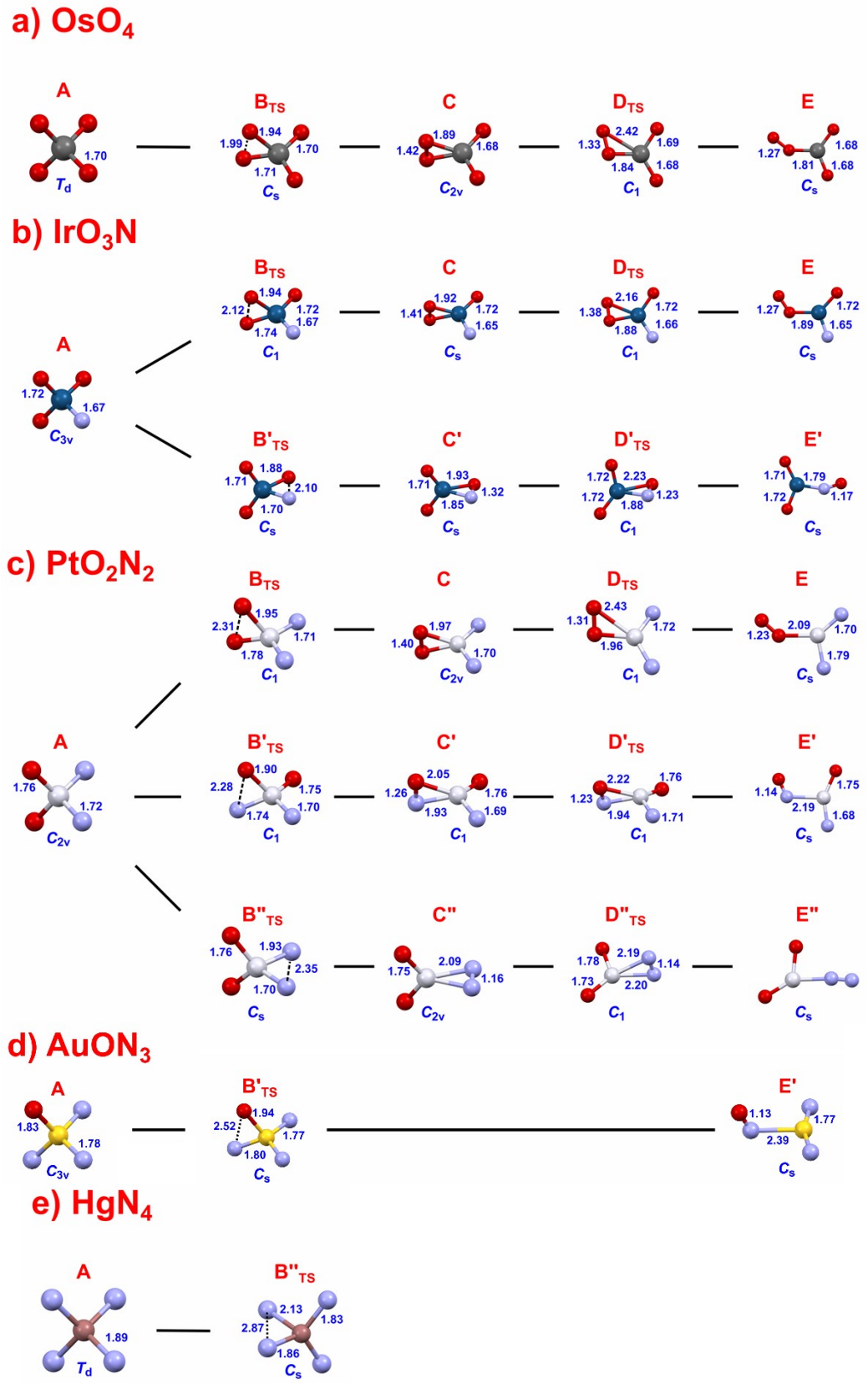


Figure S2. Equilibrium structures corresponding to stationary points constituting reaction paths of dissociation of their diatomic ligands (O_2, NO or N_2) from isomers containing metal atoms at the highest formal oxidation step (**A**) - **neutral molecules.** Molecular symmetry and chosen interatomic distances [Å] are shown. Isomers labelling was described in *Additional explanations/Structure labelling* section of this *Supporting Information*. Molecular structures were obtained from the DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (For each structure computational method is indicated in detail in *Appendix S1*). If there is a lack of structure on the figure, we were unable to optimize some of the structures with any of these methods. OsO_4 and IrO_3N structures we quote for our previous work [1].

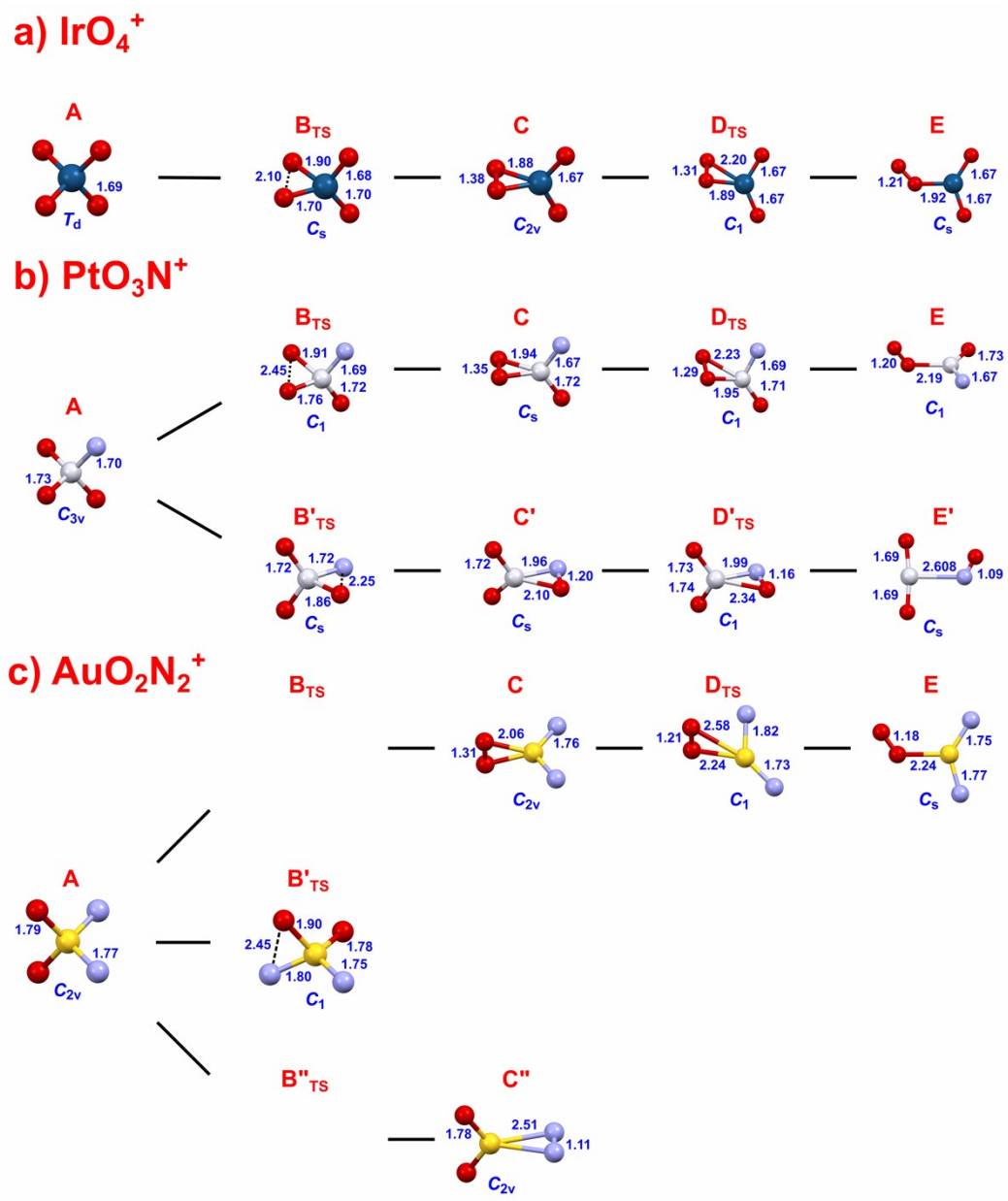


Figure S3. Equilibrium structures corresponding to stationary points constituting reaction paths of dissociation of their diatomic ligands (O_2, NO or N_2) from isomers containing metal atoms at the highest formal oxidation step (**A**) - **cationic molecules.** Molecular symmetry and chosen interatomic distances [Å] are shown. Isomers labelling was described in *Additional explanations/Structure labelling* section of this *Supporting Information*. Molecular structures were obtained from the DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (For each structure computational method is indicated in detail in *Appendix S1*). If there is a lack of structure on the figure, we were unable to optimize some of the structures with any of these methods.

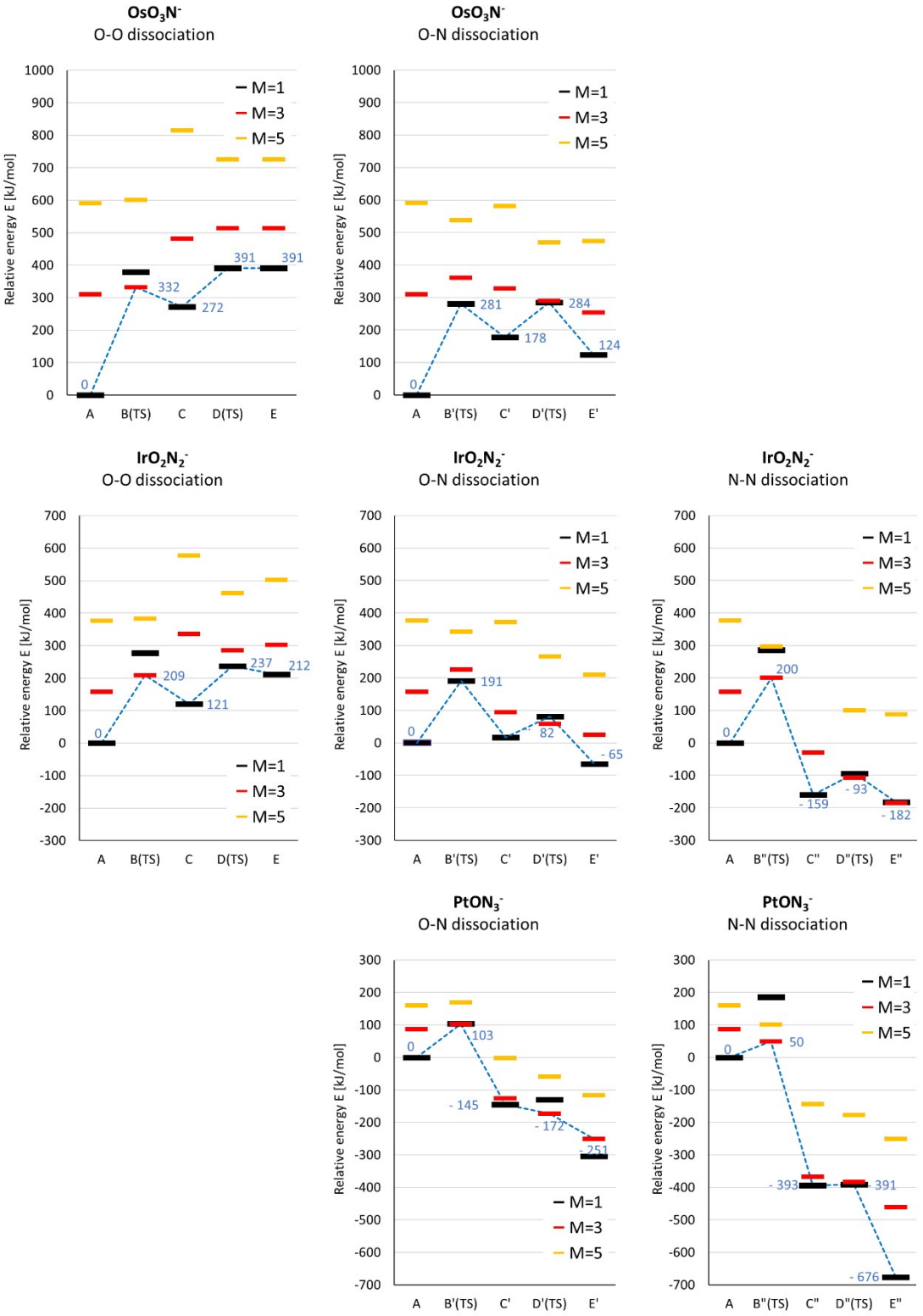
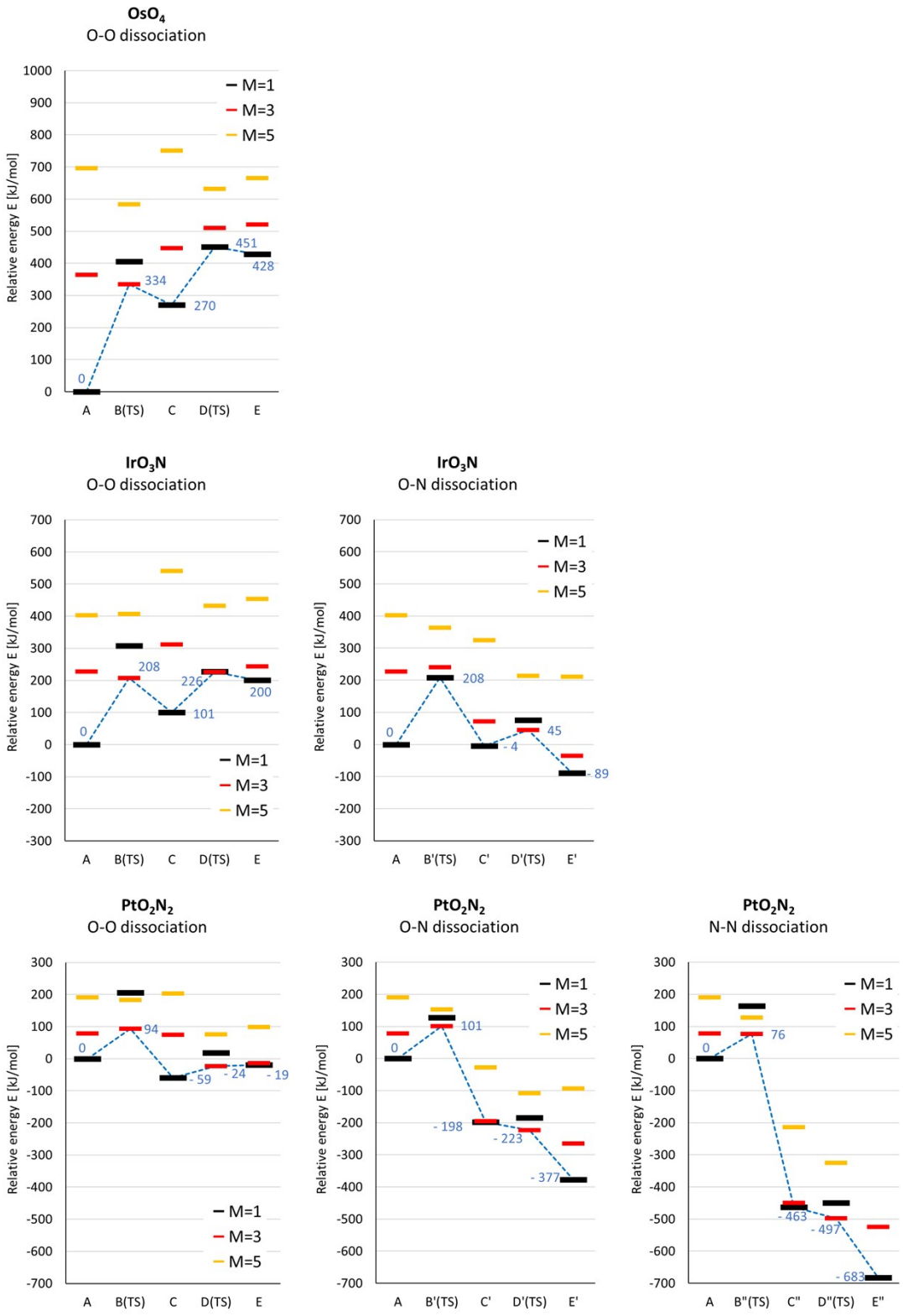


Figure S4. Relative potential energies of minimum energy and transition state (TS) equilibrium geometries for reactions of dissociations of diatomic ligands from **A** isomers containing metal atom at the highest formal oxidation state (formal $5d^0$ electron configuration) of **investigated anionic molecules.** Equilibrium geometries were obtained from DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (For each structure computational method is indicated in detail in *Appendix S1*). All equilibrium structures were singlets. For these structures single-point energies at DFT/ZORA(M06-L) level of theory were calculated for other electronic multiplicities (M). Blue dotted line and the energy values given on the graph are always for electronic state of the lowest energy. Isomers labelling was described in *Additional explanations/Structure labelling* section of this *Supporting Information*.



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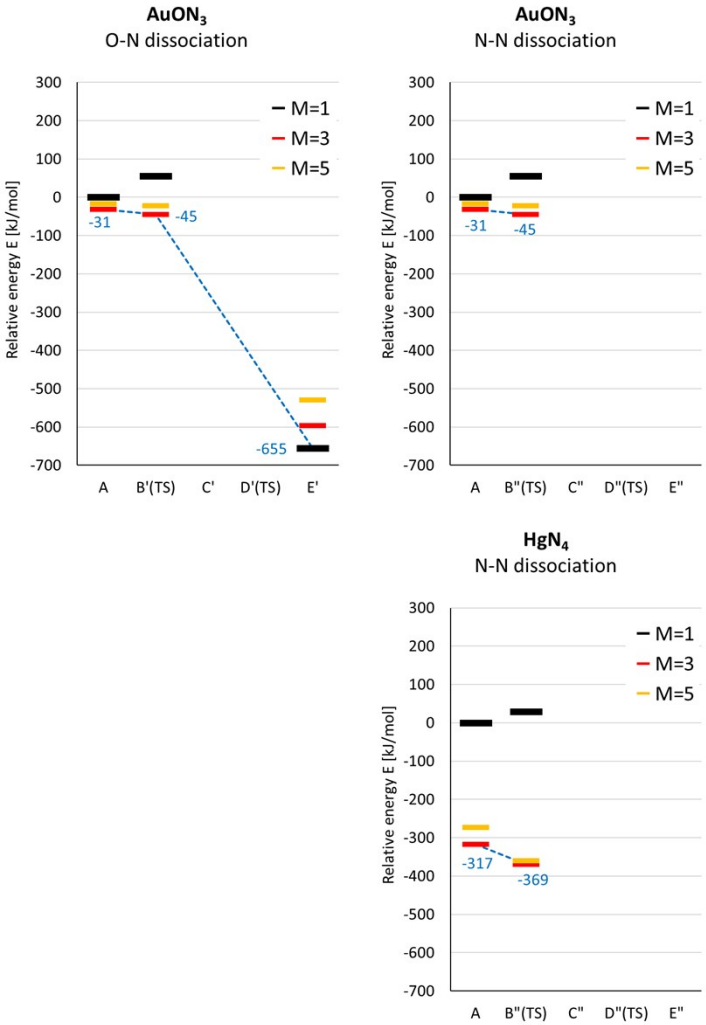


Figure S5. Relative potential energies of minimum energy and transition state (TS) equilibrium geometries for reactions of dissociations of diatomic ligands from **A** isomers containing metal atom at the highest formal oxidation state (formal $5d^0$ electron configuration) of **investigated neutral molecules.** Equilibrium geometries were obtained from DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (For each structure computational method is indicated in detail in *Appendix S1*). All equilibrium structures were singlets. For these structures single-point energies at DFT/ZORA(M06-L) level of theory were calculated for other electronic multiplicities (M). Blue dotted line and the energy values given on the graph are always for electronic state of the lowest energy. Isomers labelling was described in *Additional explanations/Structure labelling* section of this *Supporting Information*. Data for OsO_4 and IrO_3N structures we quote for our previous work [1].

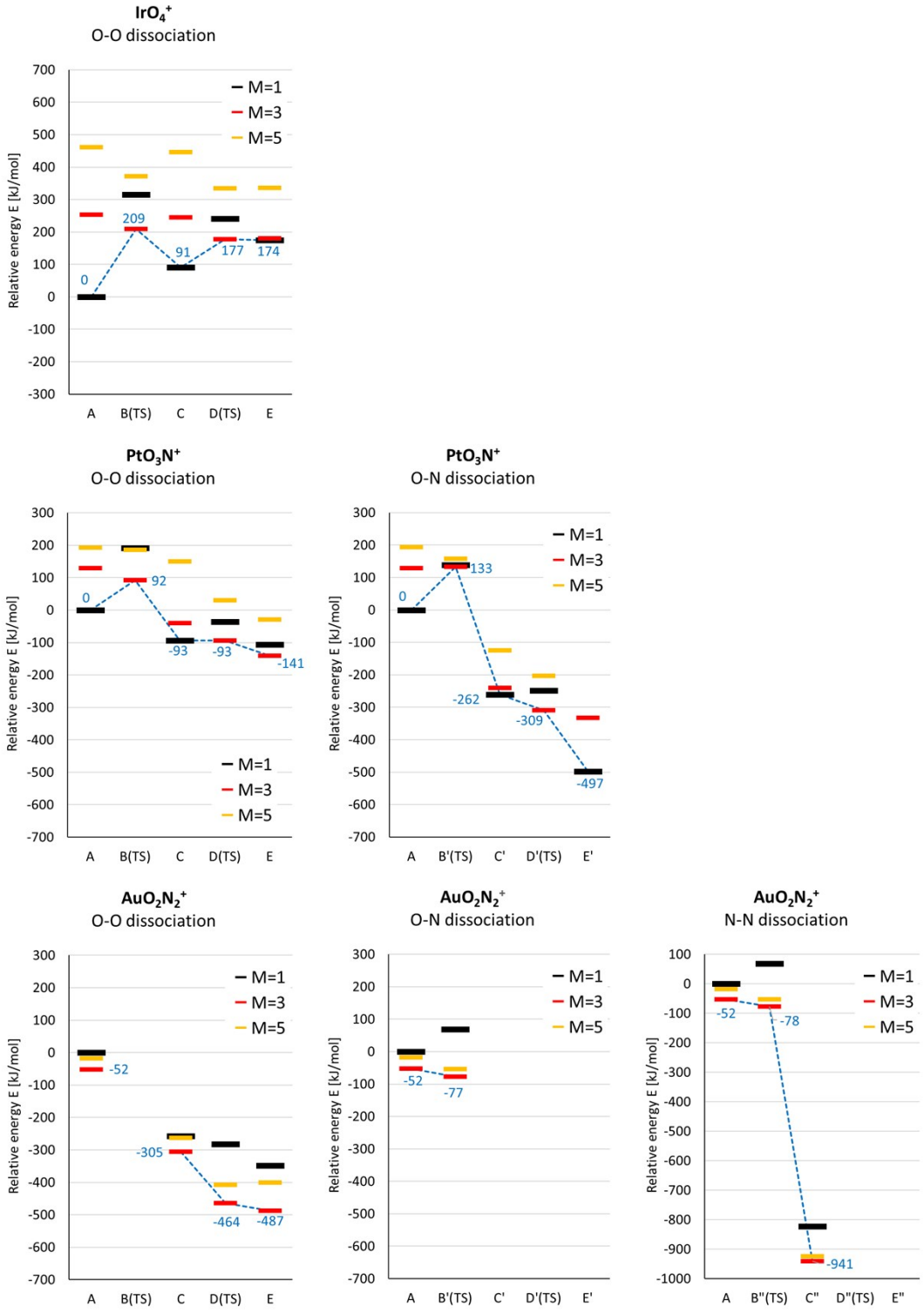


Figure S6. Relative potential energies of minimum energy and transition state (TS) equilibrium geometries for reactions of dissociations of diatomic ligands from **A** isomers containing metal atom at the highest formal oxidation state (formal $5d^0$ electron configuration) of **investigated cationic molecules.** Equilibrium geometries were obtained from DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (For each structure computational method is indicated in detail in *Appendix S1*). All equilibrium structures were singlets. For these structures single-point energies at DFT/ZORA(M06-L) level of theory were calculated for other electronic multiplicities (M). Blue dotted line and the energy values given on the graph are always for electronic state of the lowest energy. Isomers labelling was described in *Additional explanations/Structure labelling* section of this *Supporting Information*.

OsO_4 – dissociation of O_2

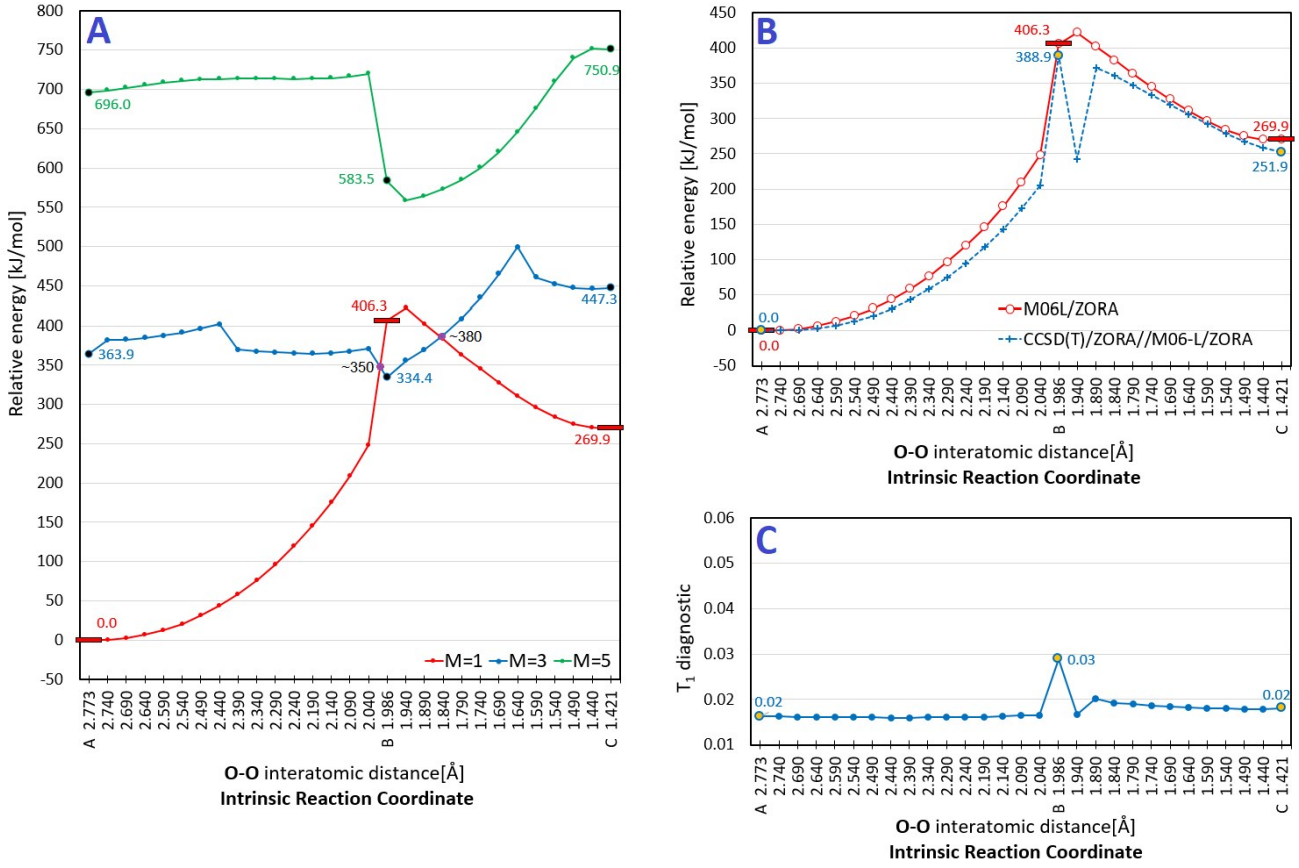


Figure S7. Reaction of **dissociation of O_2 ligand** from the **OsO_4** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$OsNO_3^-$ – dissociation of O_2

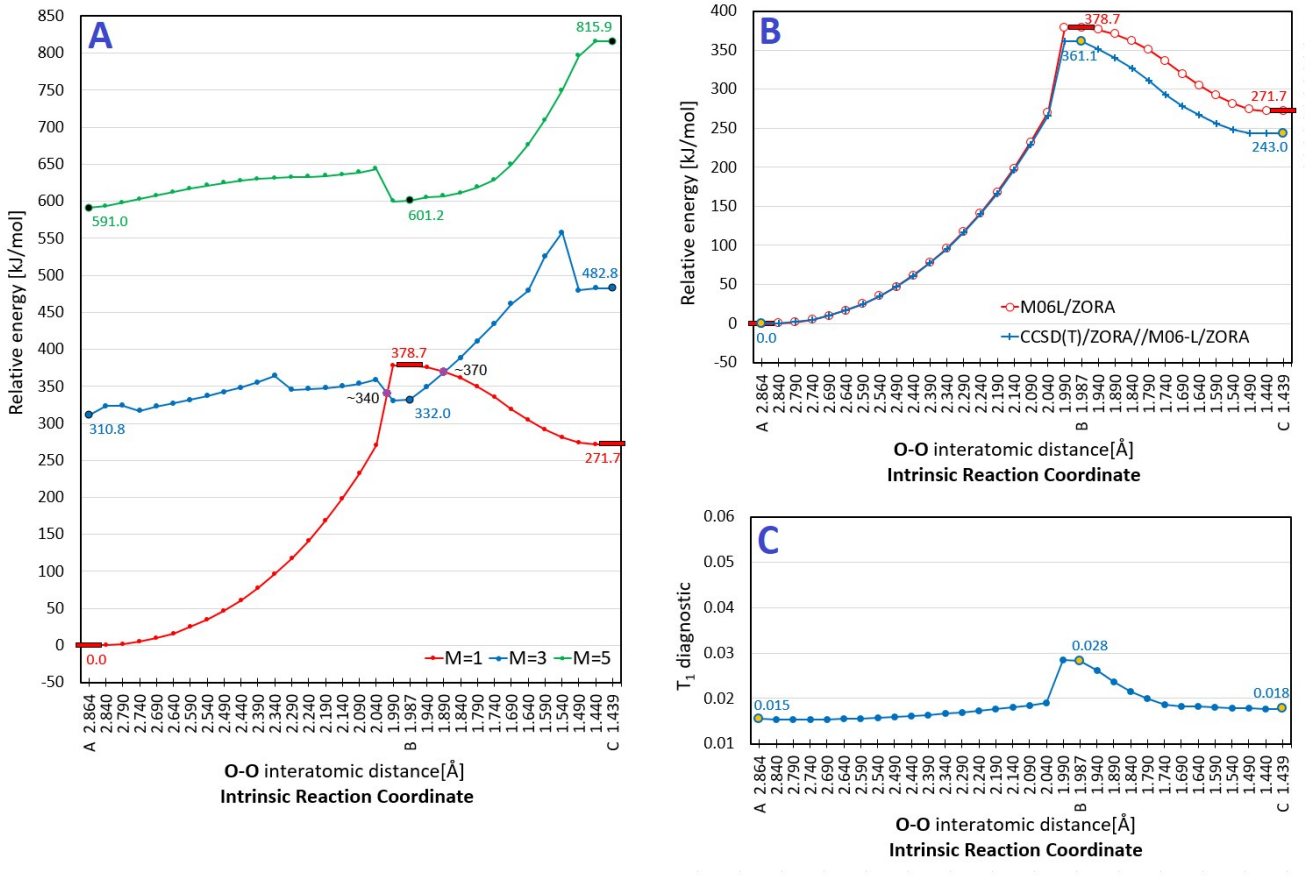


Figure S8. Reaction of **dissociation of O_2 ligand** from the **$OsNO_3^-$** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$OsNO_3^-$ – dissociation of **NO**

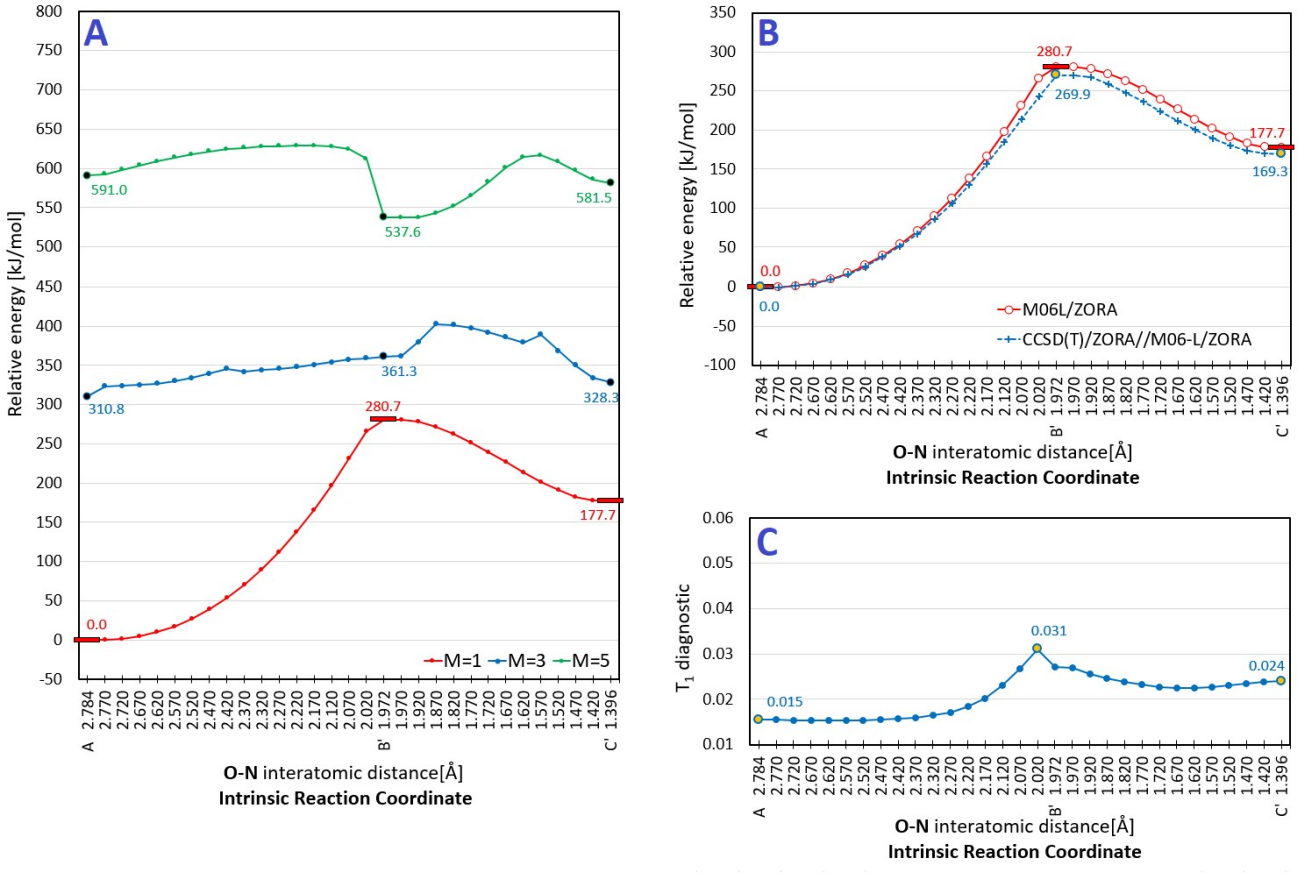


Figure S9. Reaction of **dissociation of NO ligand** from the **$OsNO_3^-$** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B'** to other minimum energy structure **C'**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

IrO_4^+ – dissociation of O_2

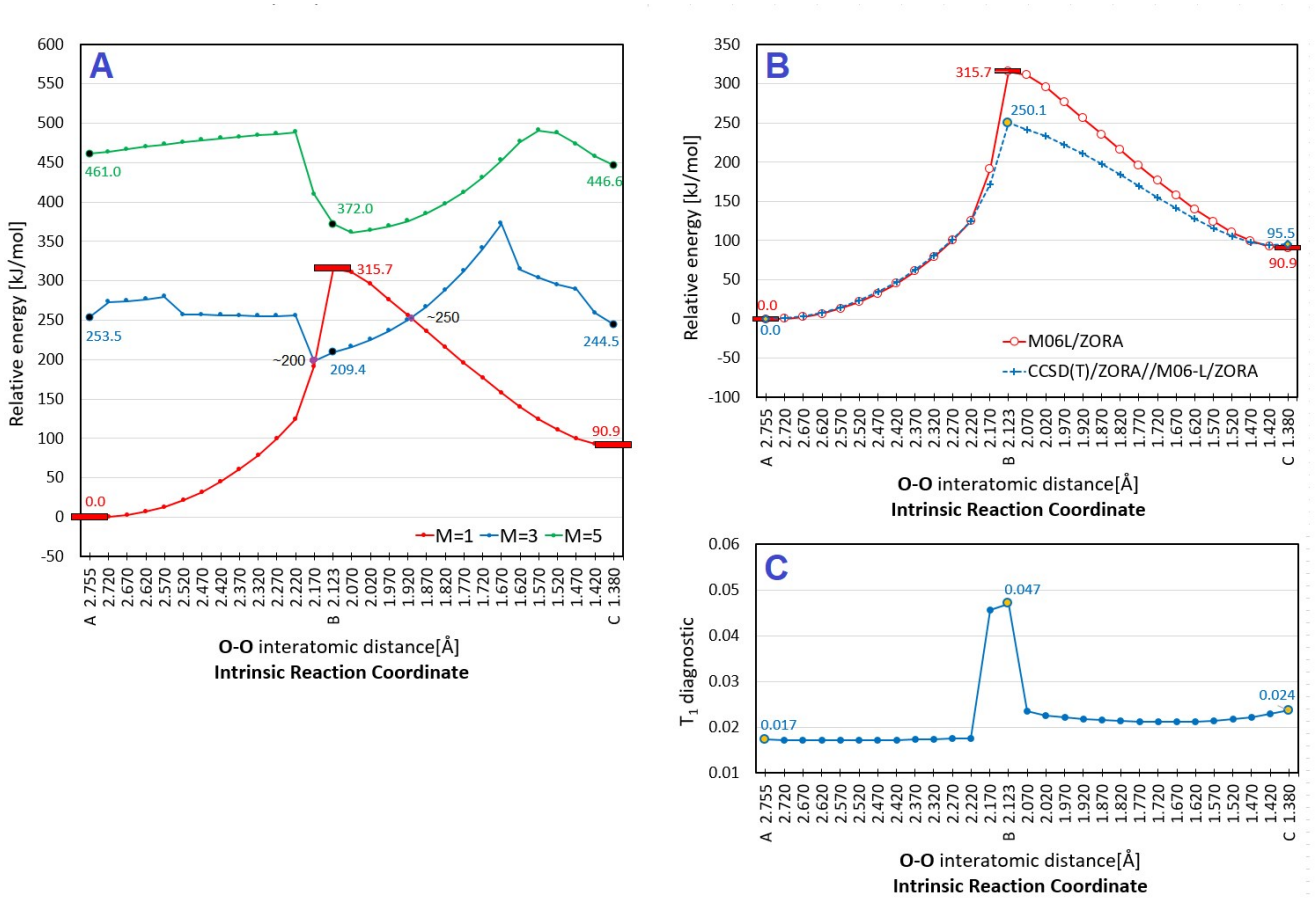


Figure S10. Reaction of **dissociation of O_2 ligand** from the **IrO_4^+** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$IrNO_3$ – dissociation of O_2

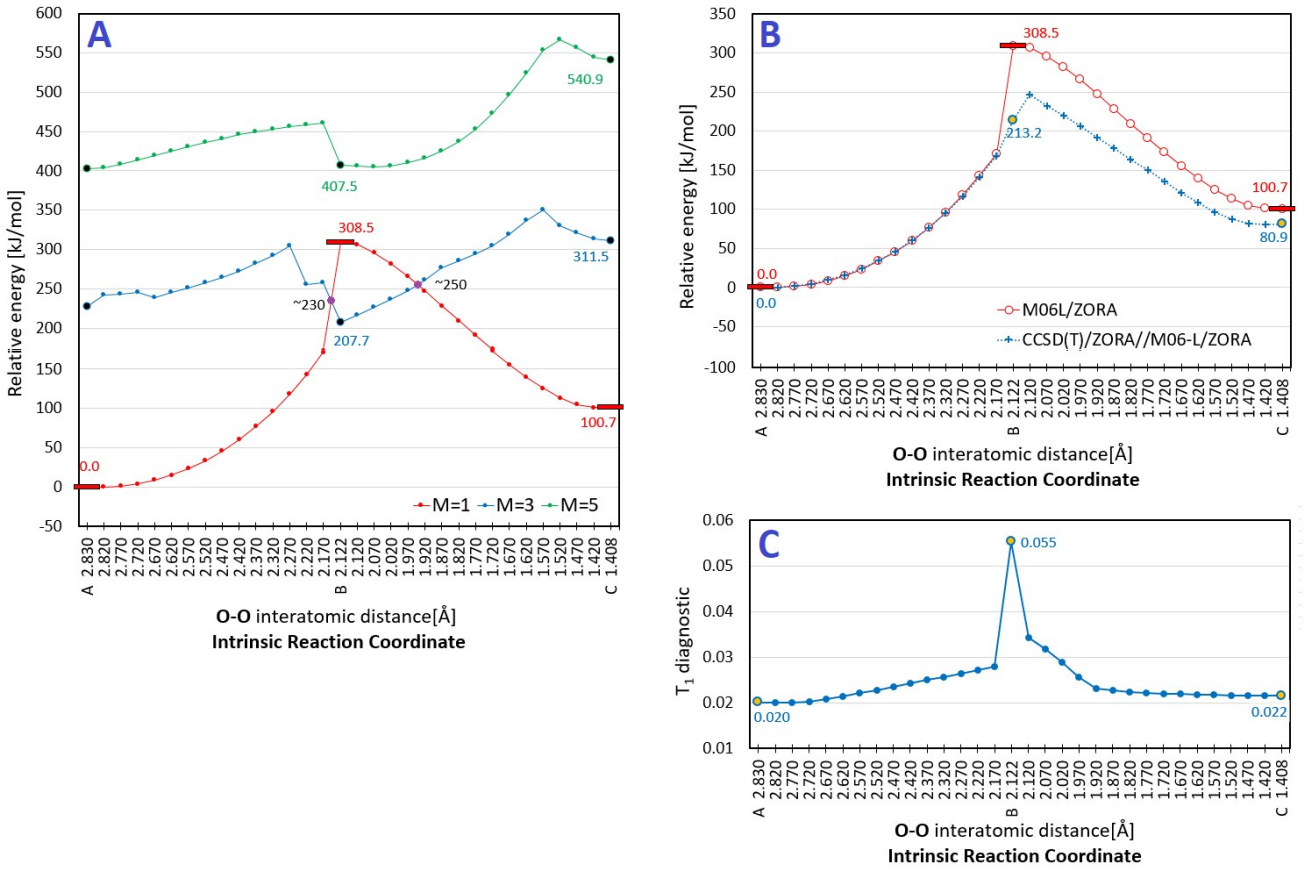


Figure S11. Reaction of **dissociation of O_2 ligand** from the **$IrNO_3$** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations. All data for $IrNO_3$ we quote for our previous work [1].

$IrNO_3$ – dissociation of **NO**

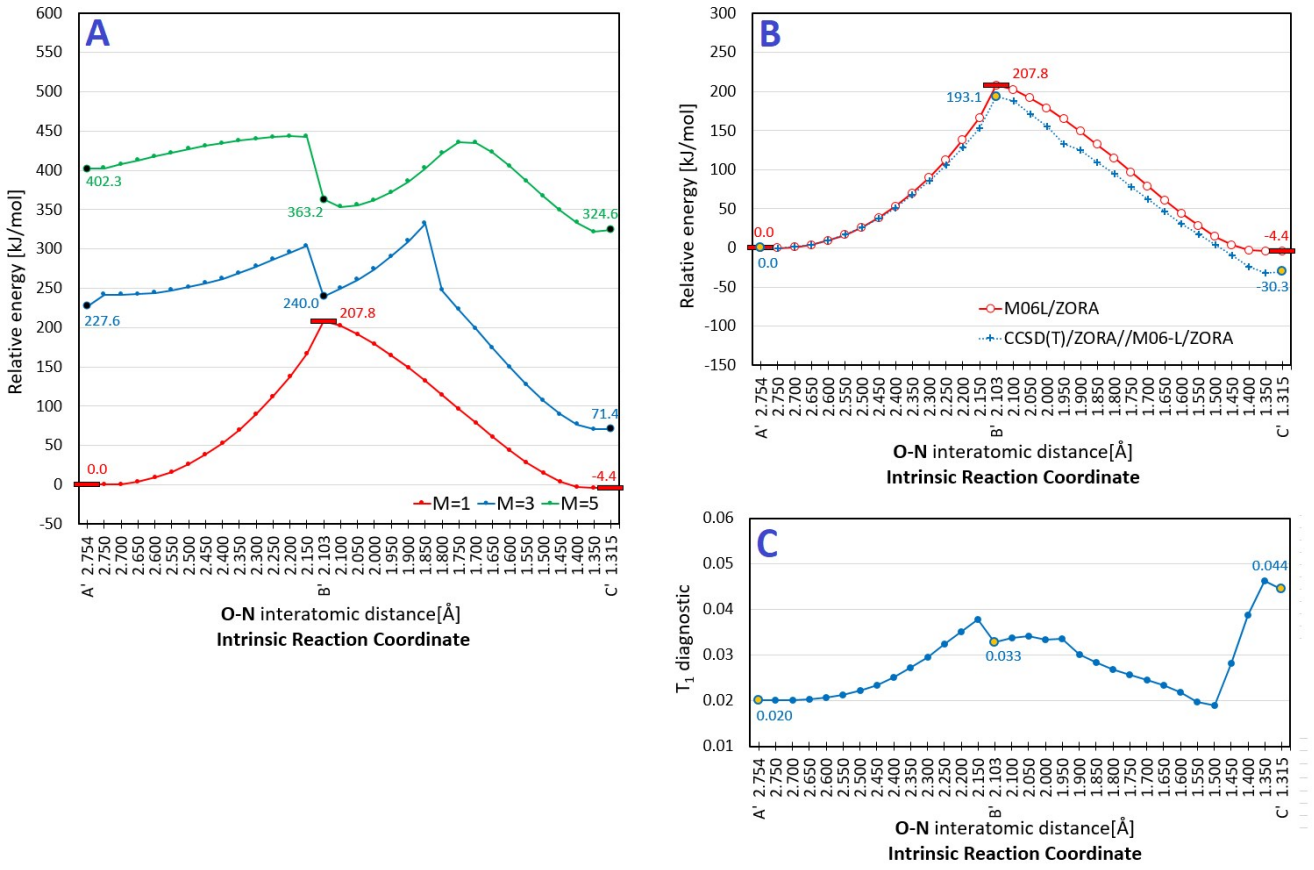


Figure S12. Reaction of **dissociation of NO ligand** from the **$IrNO_3$** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B'** to other minimum energy structure **C'**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations. All data for $IrNO_3$ we quote for our previous work [1].

$IrN_2O_2^-$ – dissociation of O_2

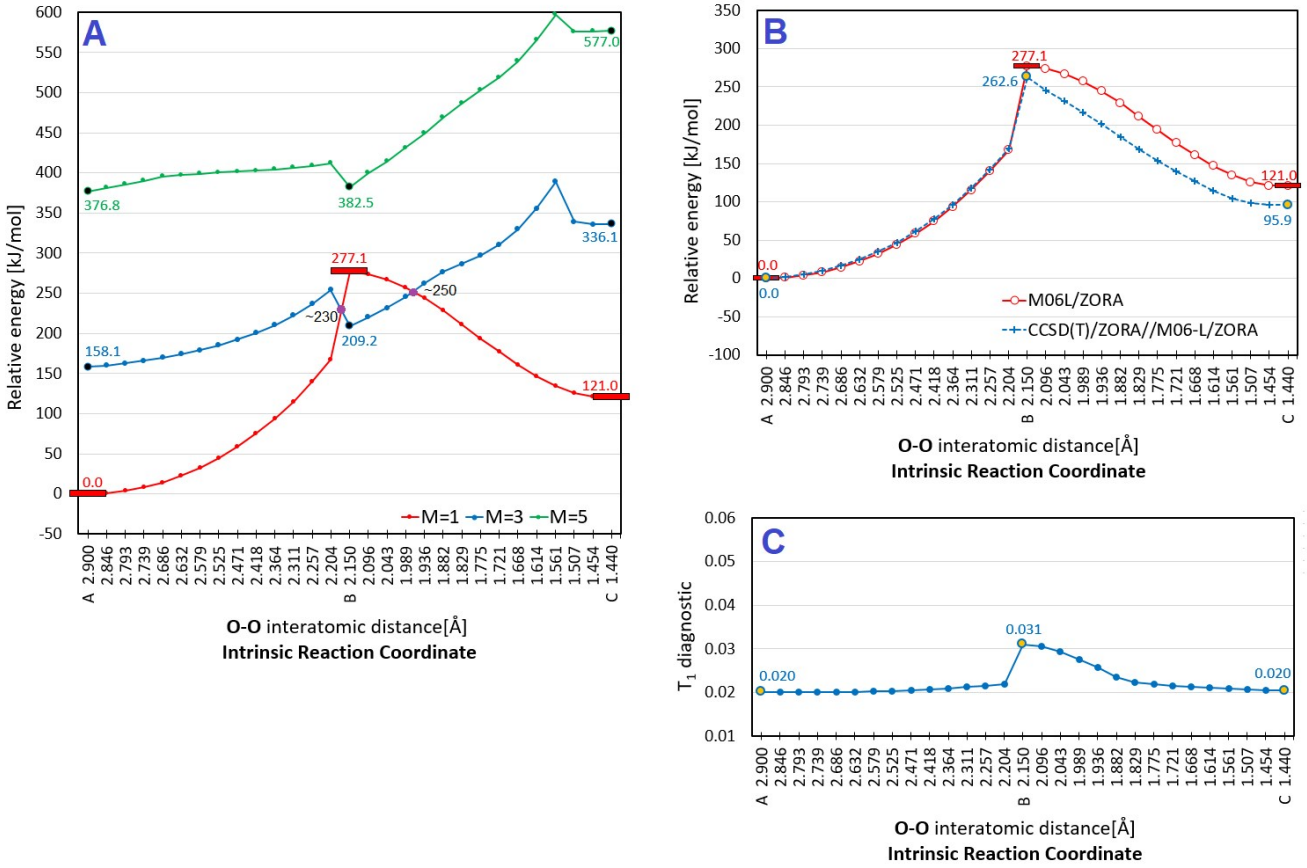


Figure S13. Reaction of **dissociation of O_2 ligand** from the **$IrN_2O_2^-$** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$IrN_2O_2^-$ – dissociation of **NO**

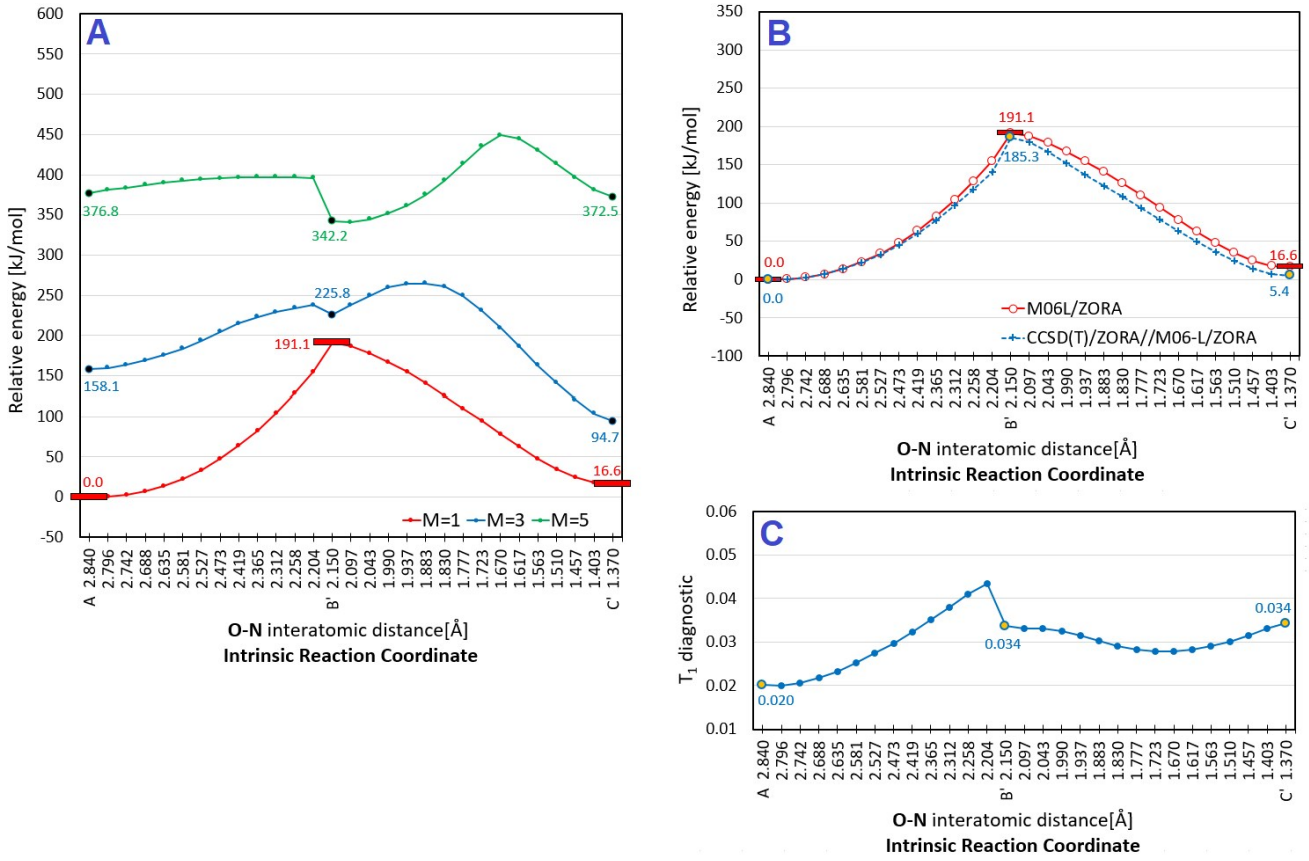


Figure S14. Reaction of **dissociation of NO ligand** from the IrN_2O_2 molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B'** to other minimum energy structure **C'**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$IrN_2O_2^-$ – dissociation of N_2

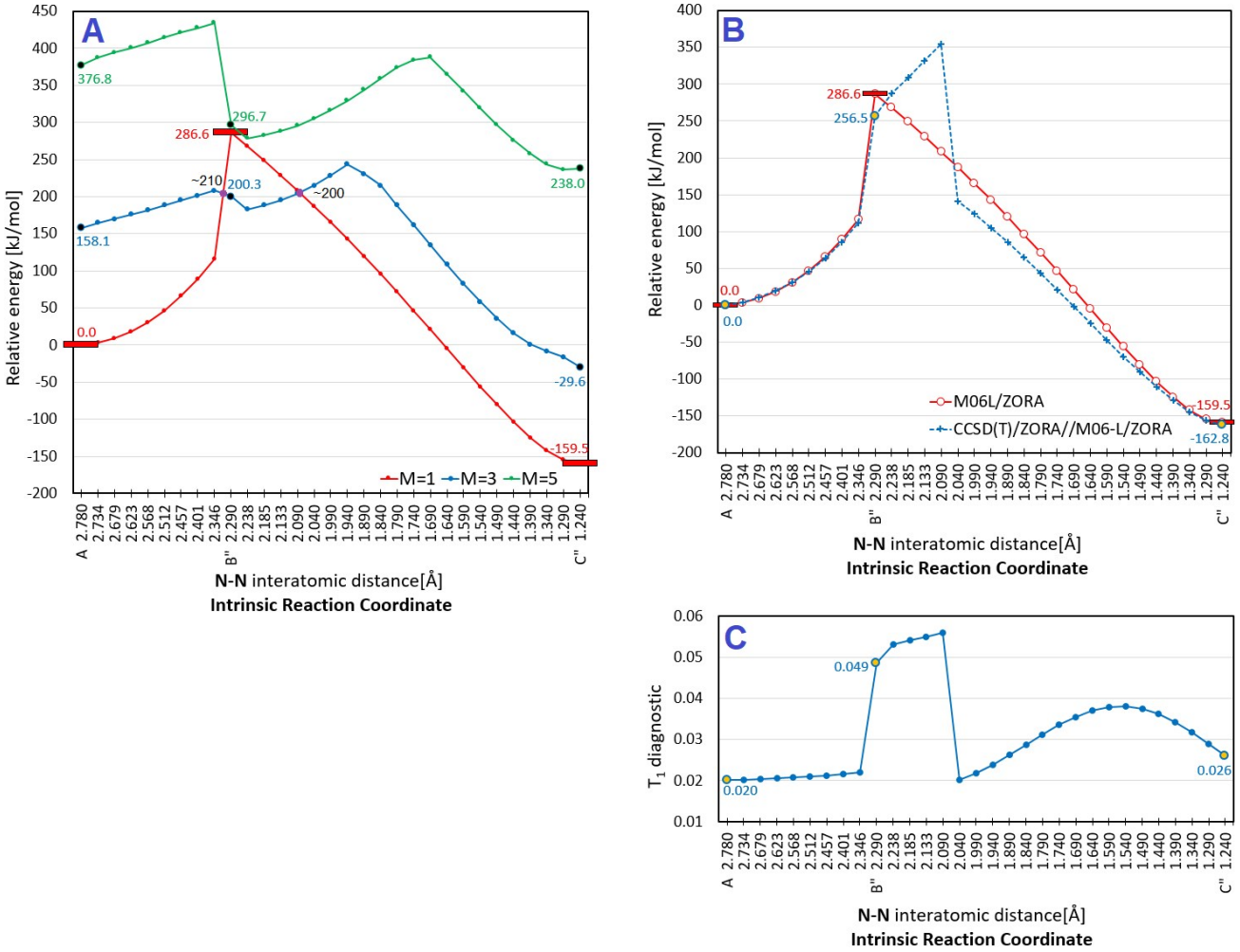


Figure S15. Reaction of **dissociation of N_2 ligand** from the $IrN_2O_2^-$ molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B"** to other minimum energy structure **C"**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

PtO_4^{2+} – dissociation of O_2

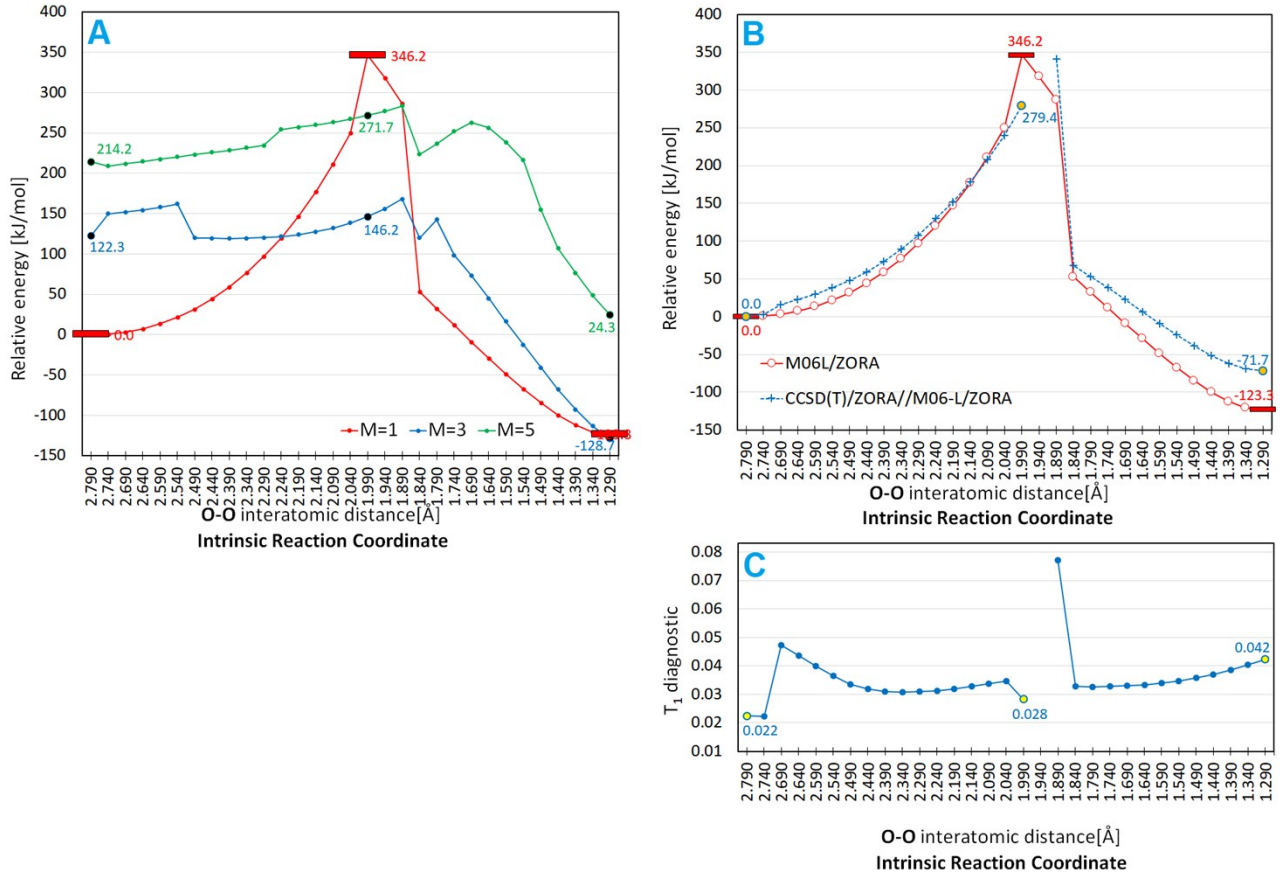


Figure S16. Reaction of **dissociation of O_2 ligand** from the PtO_4^{2+} molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero. For a few points of path CCSD(T)/ZORA single-point energy computations were failed due to some numerical difficulties probably caused by the strong multi-reference nature of these systems.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$PtNO_3^+$ – dissociation of O_2

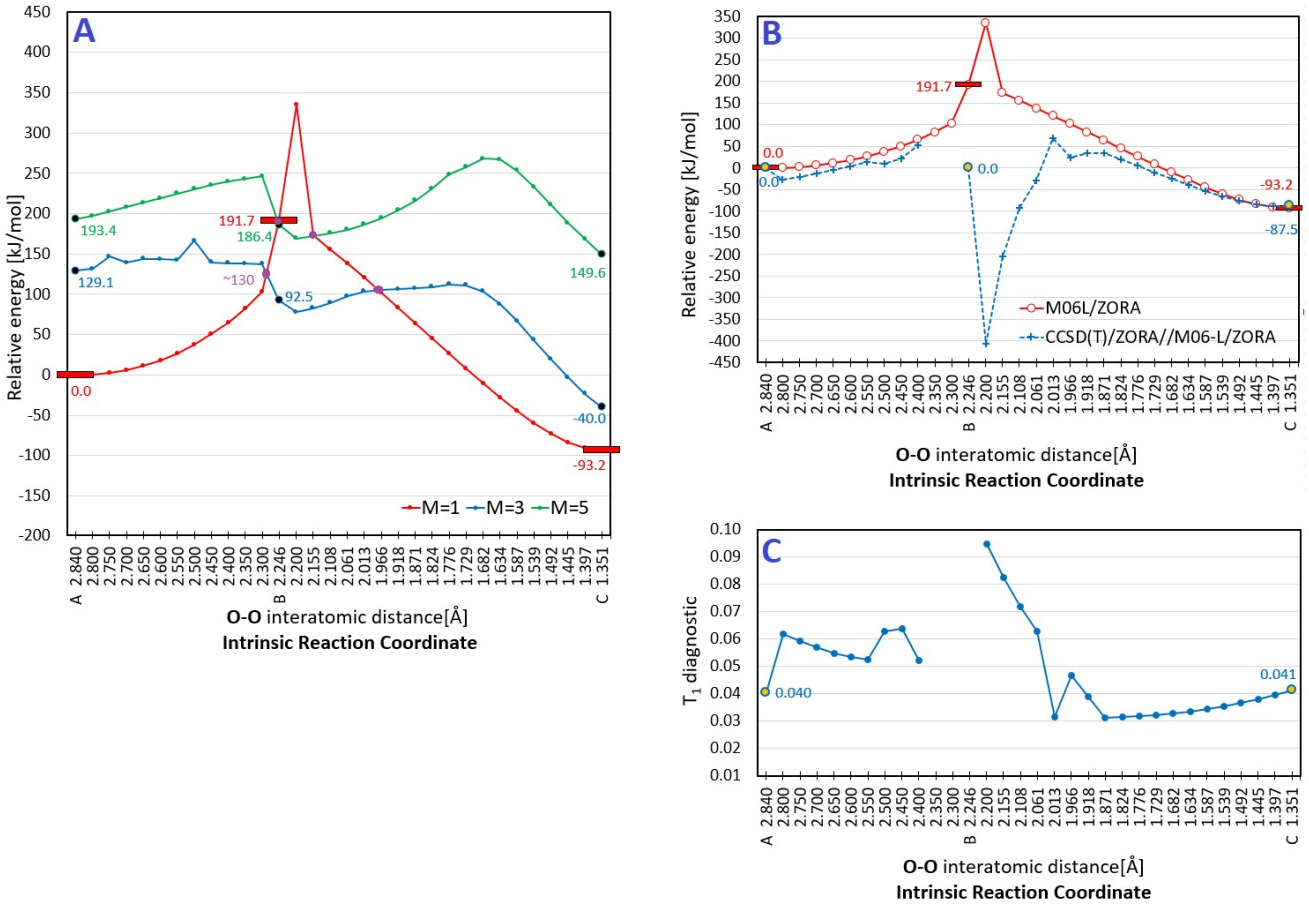


Figure S17. Reaction of **dissociation of O_2 ligand** from the **$PtNO_3^+$** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero. For a few points of path CCSD(T)/ZORA single-point energy computations were failed due to some numerical difficulties probably caused by the strong multi-reference nature of these systems.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

$PtNO_3^+$ – dissociation of **NO**

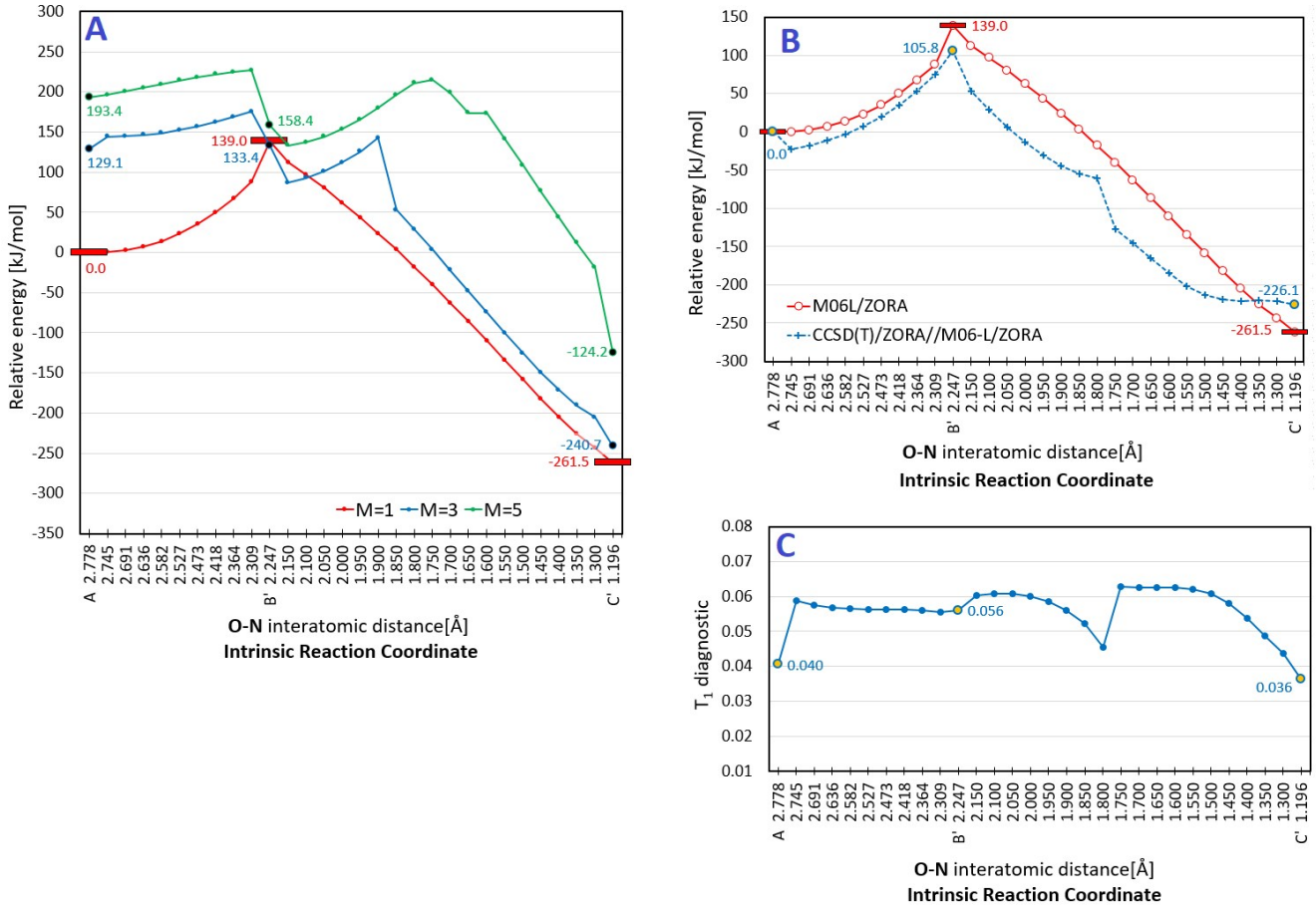


Figure S18. Reaction of **dissociation of NO ligand** from the $PtNO_3^+$ molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B'** to other minimum energy structure **C'**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

PtN_2O_2 – dissociation of O_2

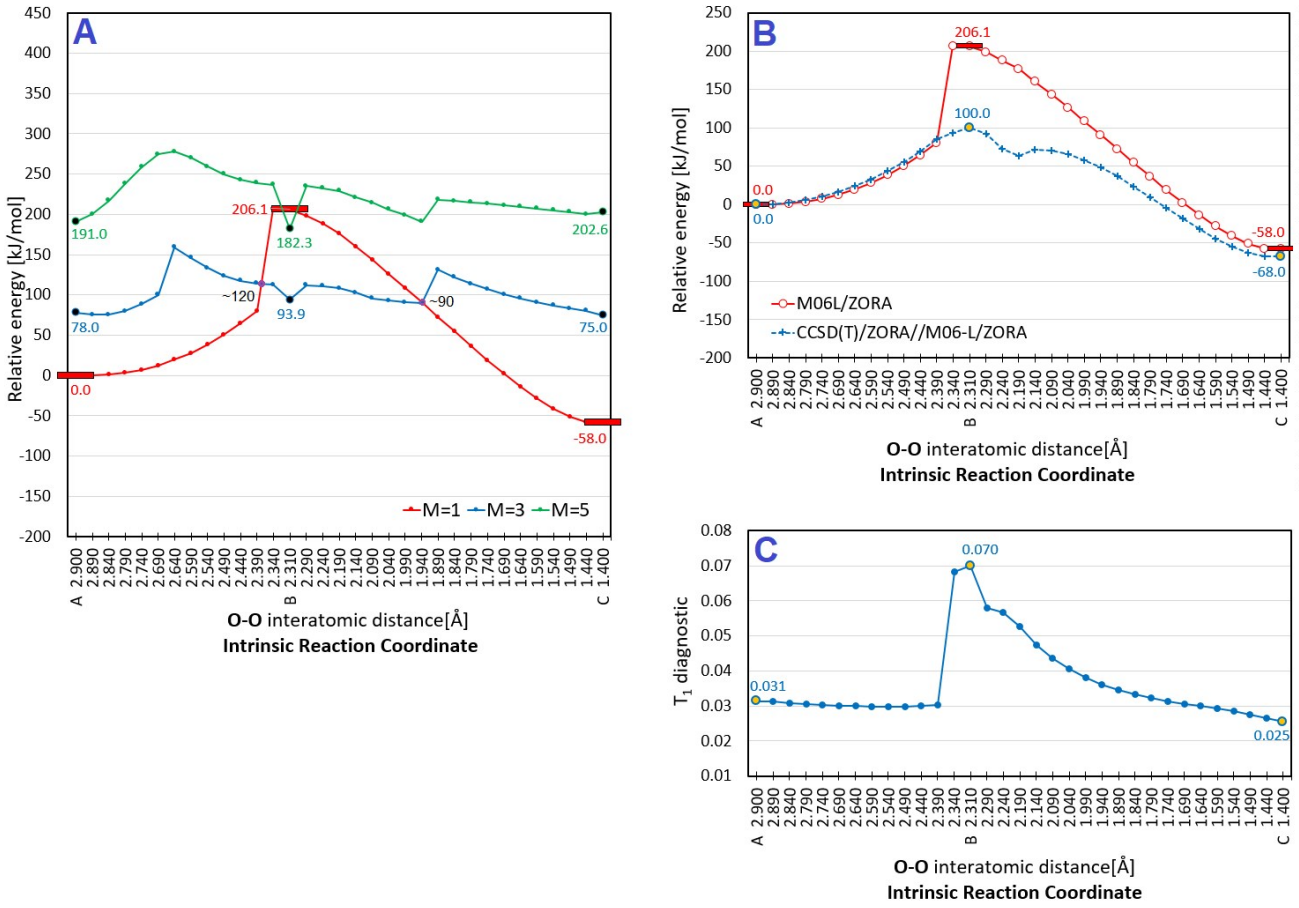


Figure S19. Reaction of **dissociation of O_2 ligand** from the **PtN_2O_2** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B** to other minimum energy structure **C**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a 0.05 Å increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

PtN_2O_2 – dissociation of NO

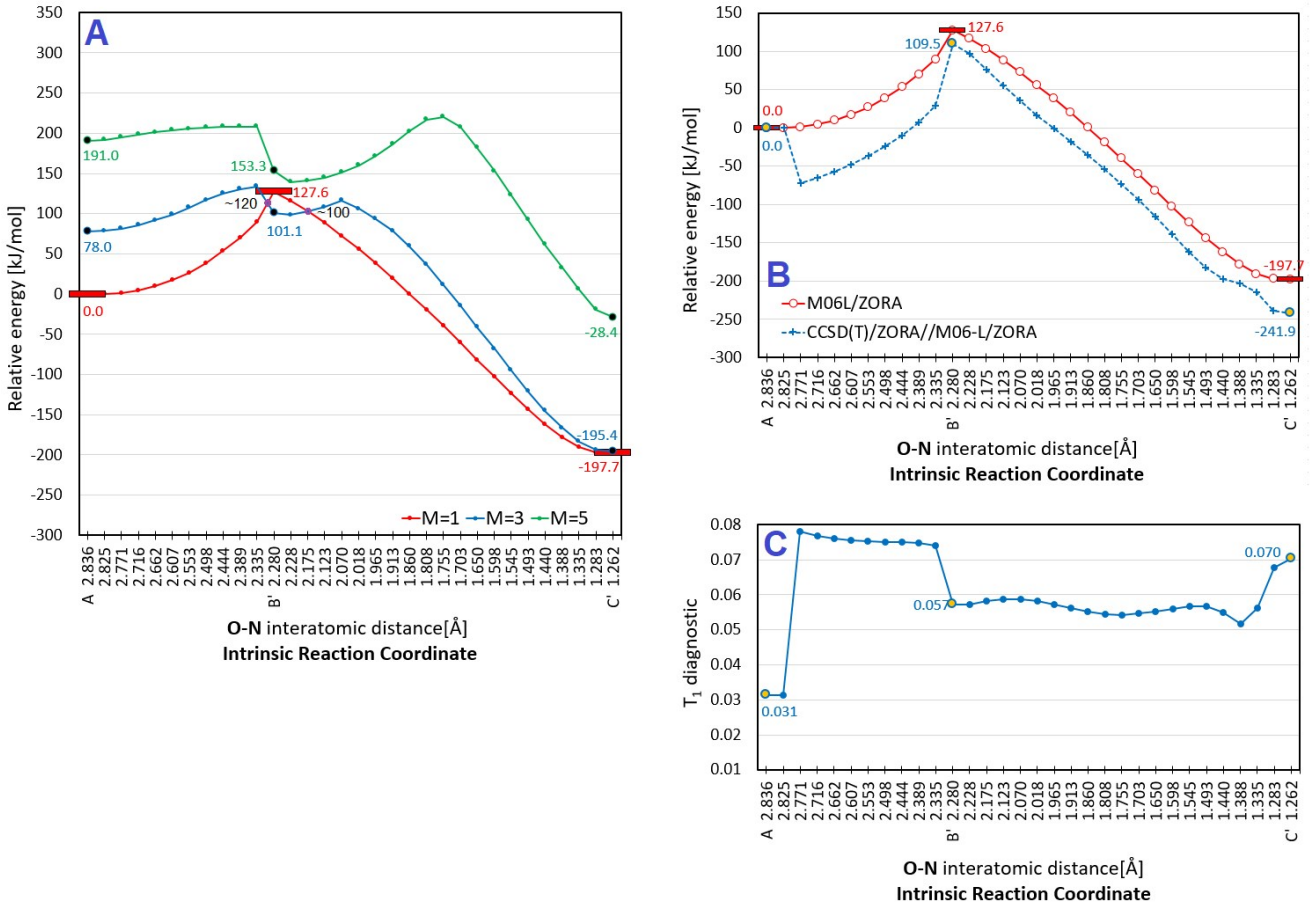


Figure S20. Reaction of **dissociation of NO ligand** from the **PtN_2O_2** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B'** to other minimum energy structure **C'**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

PtN_2O_2 – dissociation of N_2

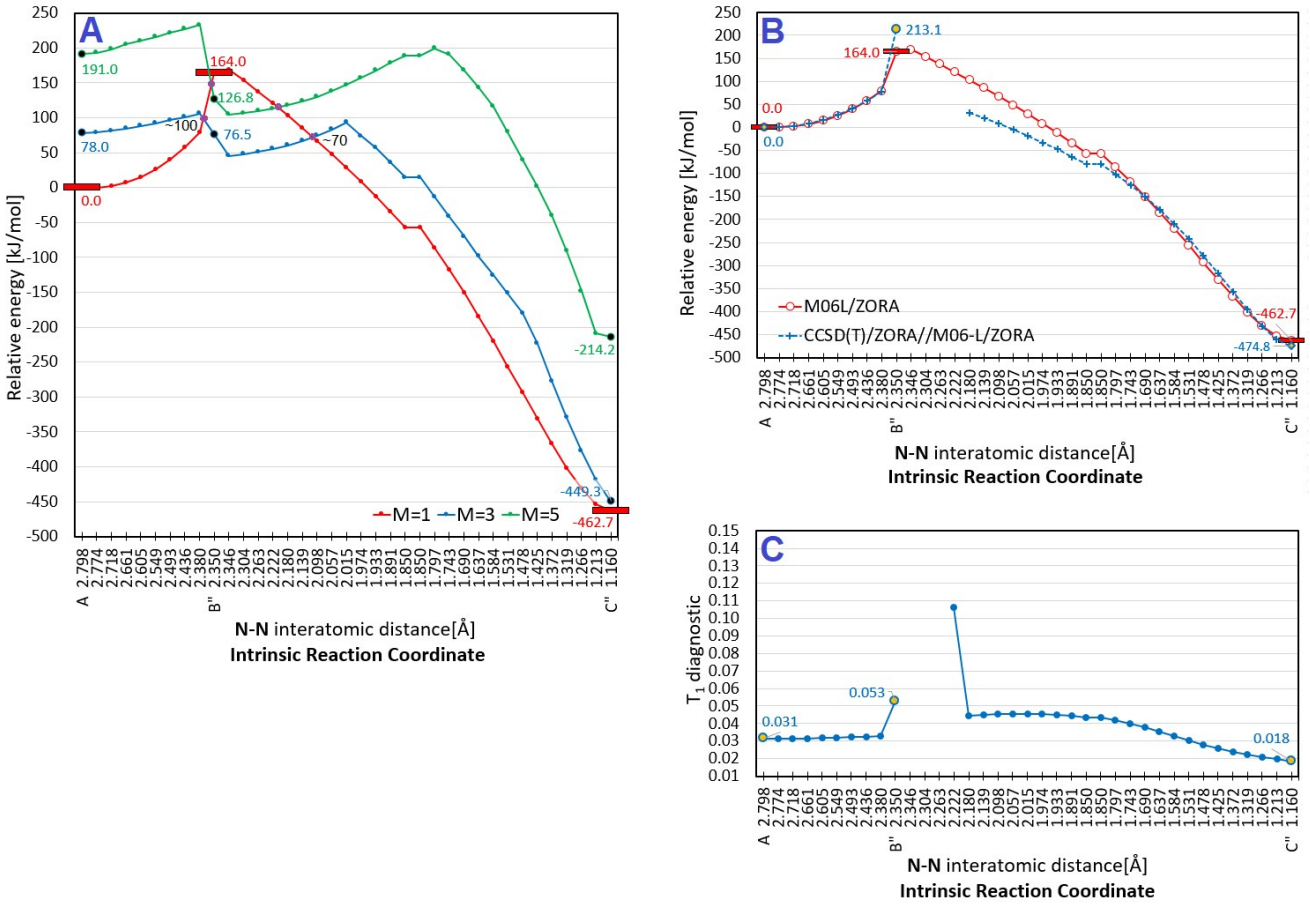


Figure S21. Reaction of **dissociation of N_2 ligand** from the **PtN_2O_2** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B"** to other minimum energy structure **C"**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero. For a few points of path CCSD(T)/ZORA single-point energy computations were failed due to some numerical difficulties probably caused by the strong multi-reference nature of these systems.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

PtN_3O^- – dissociation of NO

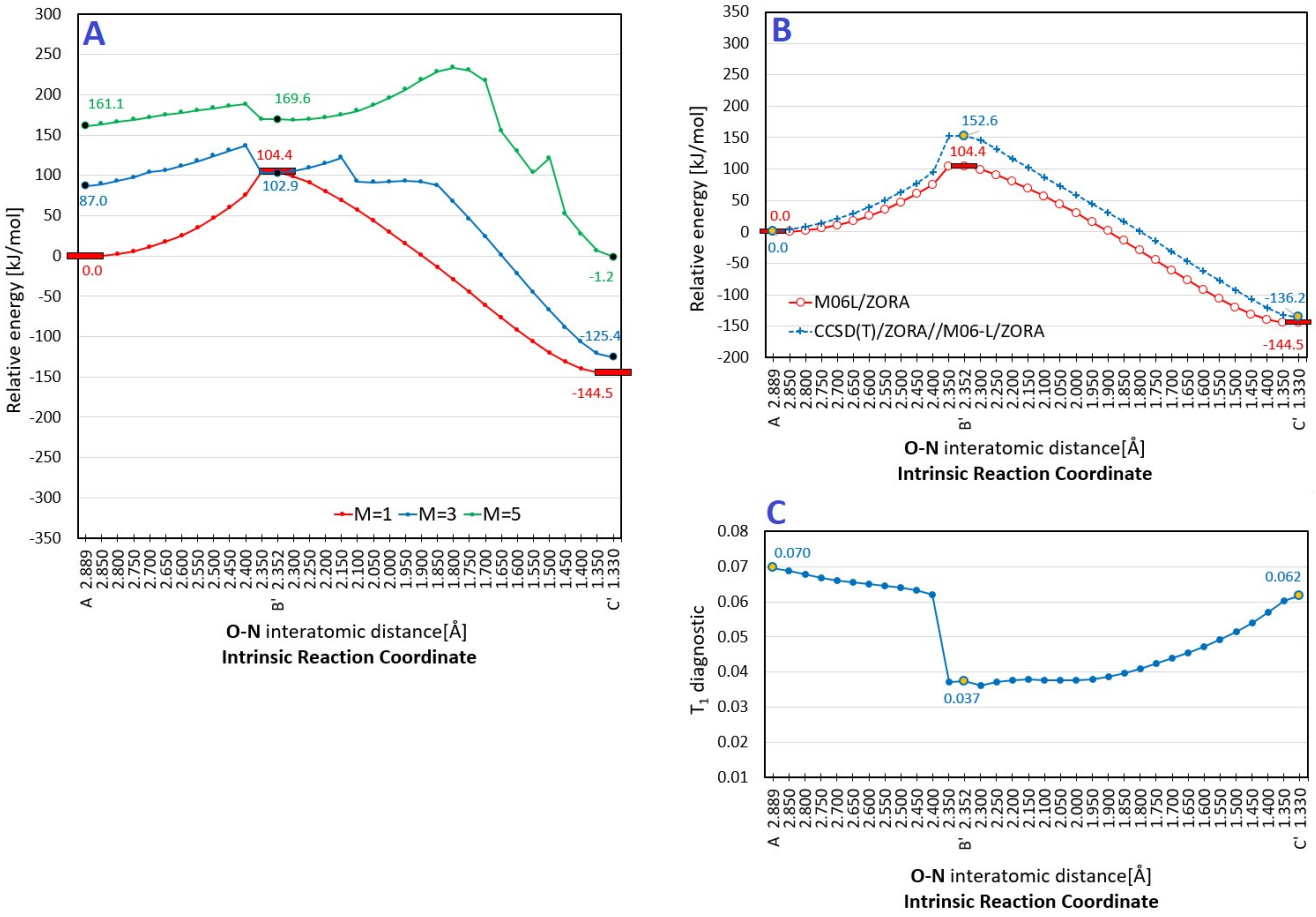


Figure S22. Reaction of **dissociation of NO ligand** from the **PtN_3O^-** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B'** to other minimum energy structure **C'**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

PtN_3O^- – dissociation of N_2

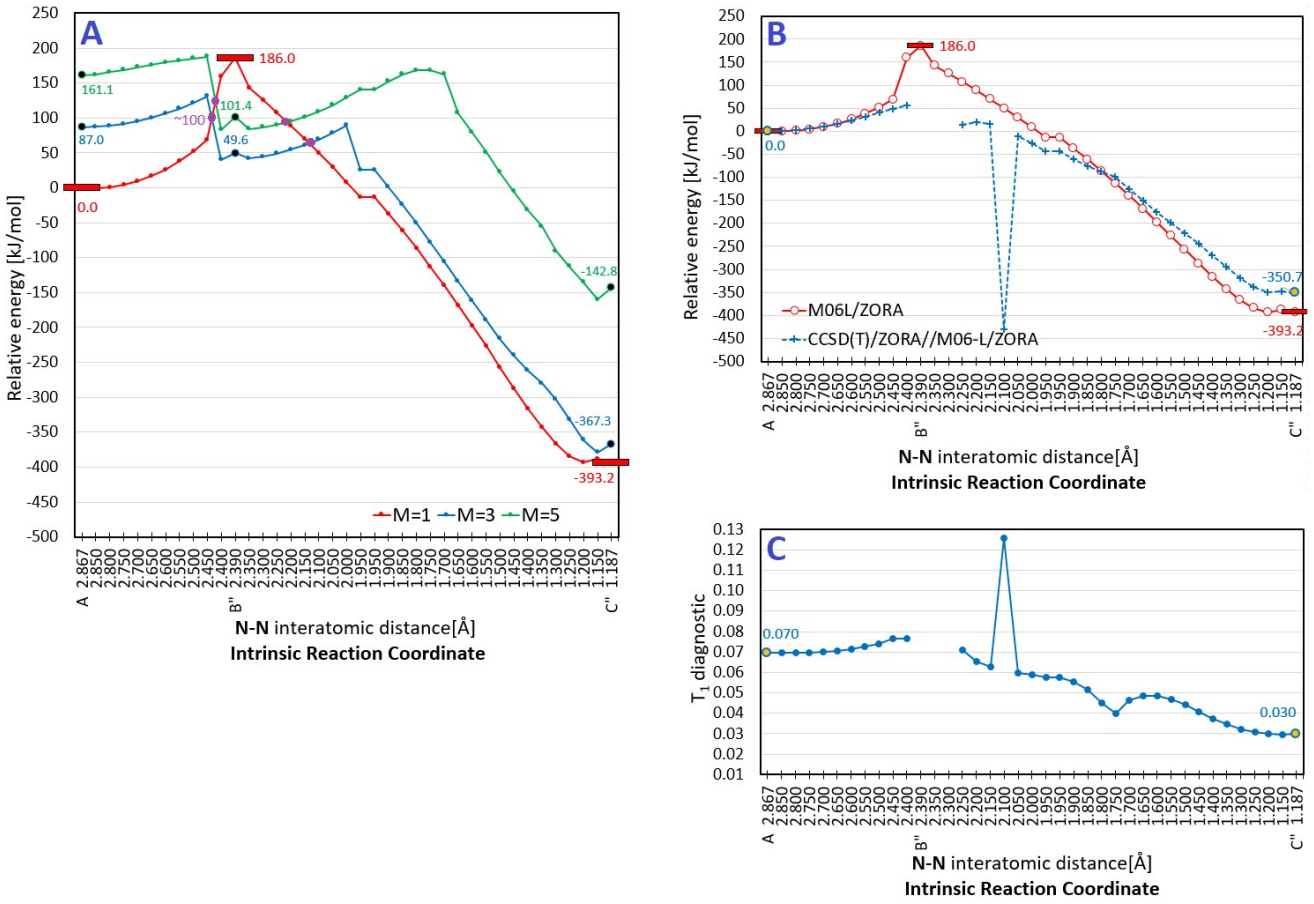


Figure S23. Reaction of **dissociation of N_2 ligand** from the **PtN_3O^-** molecule. Reaction path leads from **A** minimum structure (the highest formal oxidation state of metal atom) through transition state **B"** to other minimum energy structure **C"**. Potential energy curve corresponding to the reaction path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. Values of these bond lengths were changed step by step with a defined increment each. All shown energies ale relative: singlet-state energy of **A** isomer is set to zero. For a few points of path CCSD(T)/ZORA single-point energy computations were failed due to some numerical difficulties probably caused by the strong multi-reference nature of these systems.
A. For calculated geometries (all singlets, M=1) single-point energies were calculated also for triplet (M=3) and quintet (M=5) multiplicities to find any intersection points. **B.** Comparison of reaction energy profiles obtained from DFT/ZORA and CCSD(T)/ZORA single-point energy calculations. **C.** T_1 diagnostic values obtained for CCSD(T)/ZORA energy calculations.

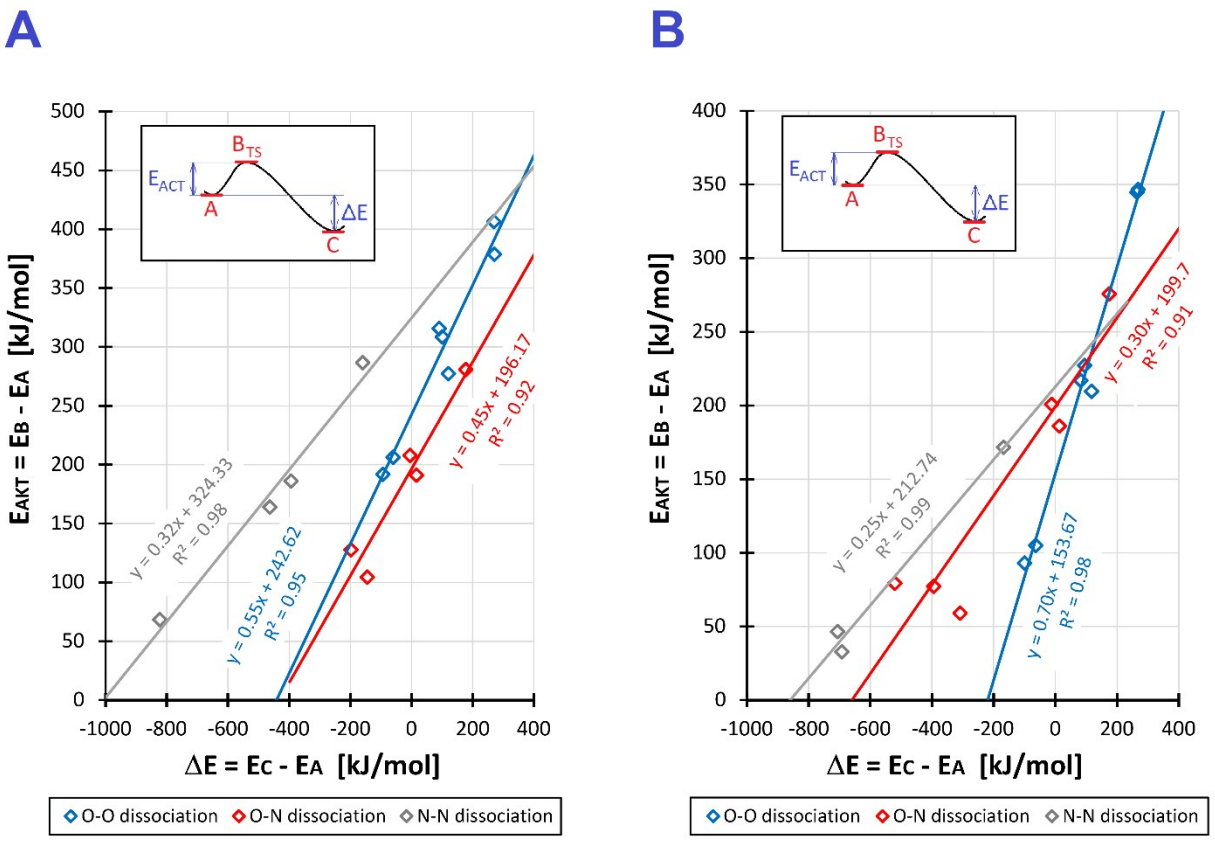


Figure S24. Testifying the validity of the Hammond's rule on investigated series of molecules: dependence between the **A→B_{TS}→C** reaction activation energy (E_{ACT}) and its energy (ΔE) for all investigated molecules: **A.** data obtained with DFT(M06-L)/ZORA approach **B.** at DFT(M06-L)/SO-ZORA level of theory. All data are divided to three families of reactions (O_2, NO, and N_2 dissociations). Linear regression trend lines with their equations and goodness of fit values (R^2) are shown. PtO_4^{2+} as the only dication was not taken under consideration.

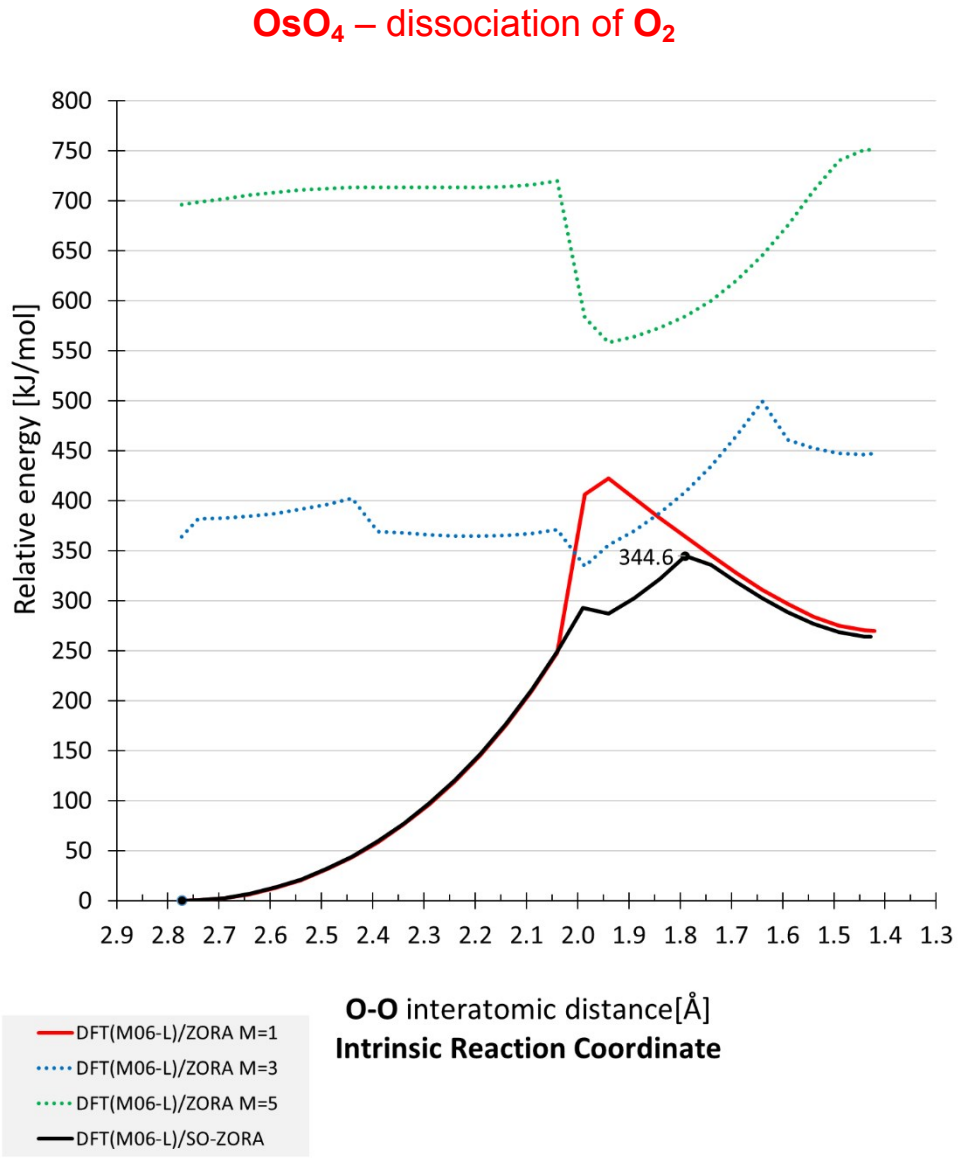


Figure S25. Reaction of **O_2 ligand** dissociation from **OsO_4** molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

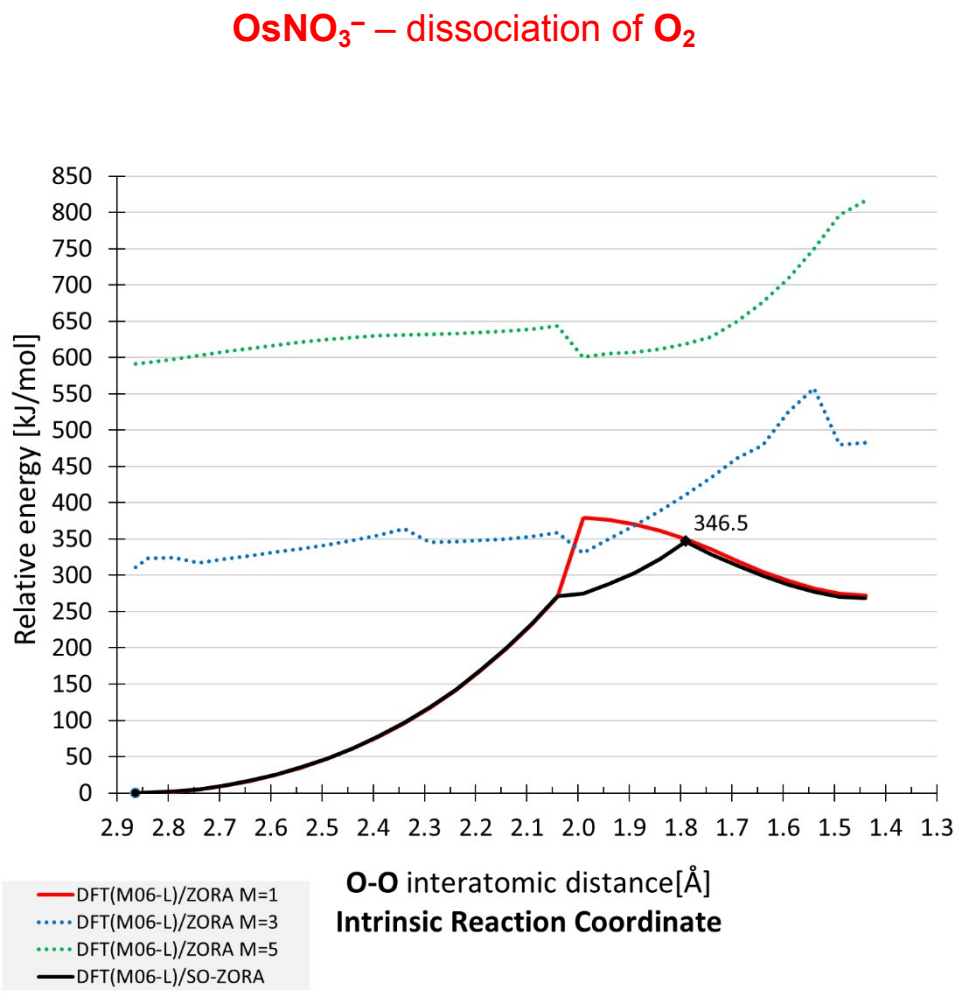


Figure S26. Reaction of **O_2 ligand** dissociation from **$OsNO_3^-$** anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

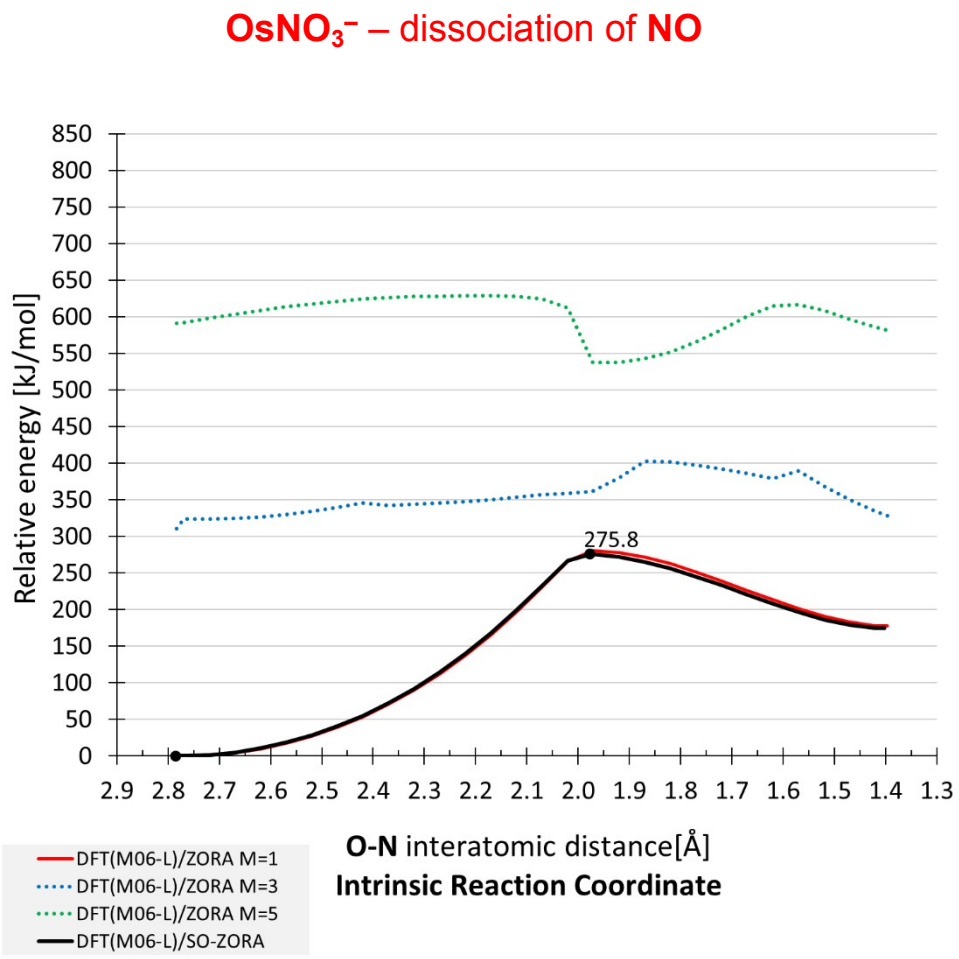


Figure S27. Reaction of **NO ligand** dissociation from **$OsNO_3^-$** anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

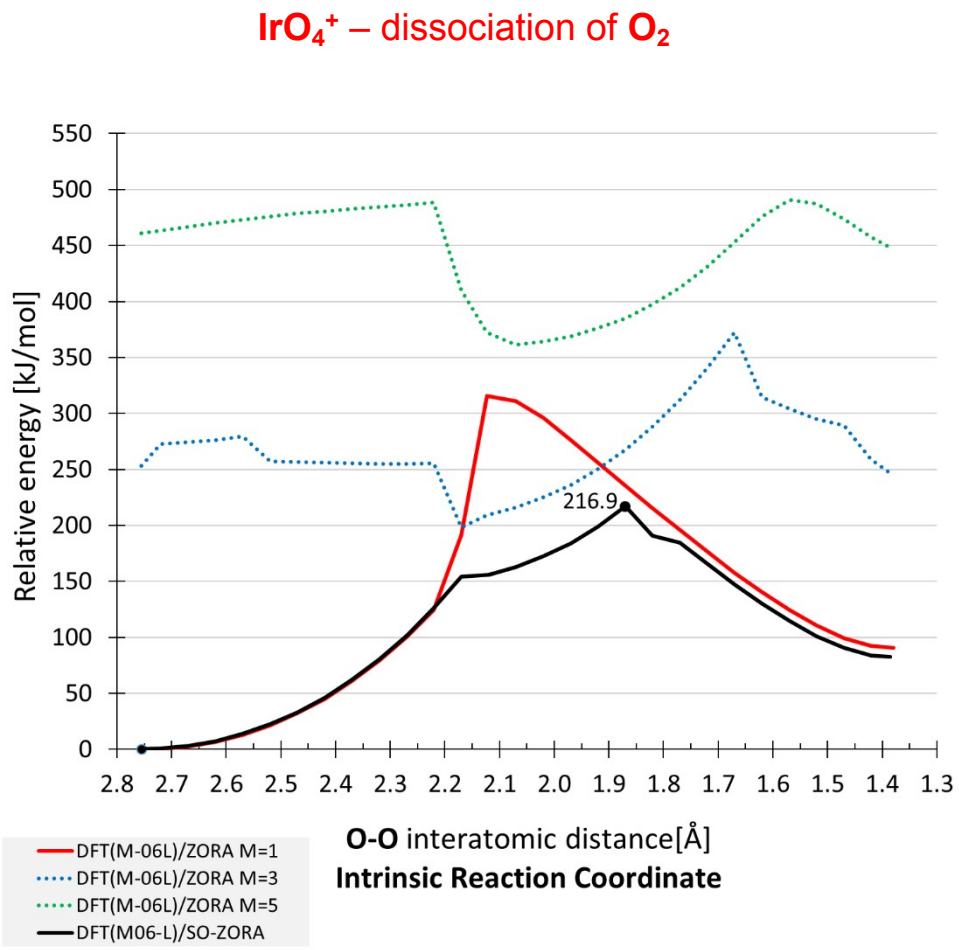


Figure S28. Reaction of O_2 **ligand** dissociation from IrO_4^+ molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

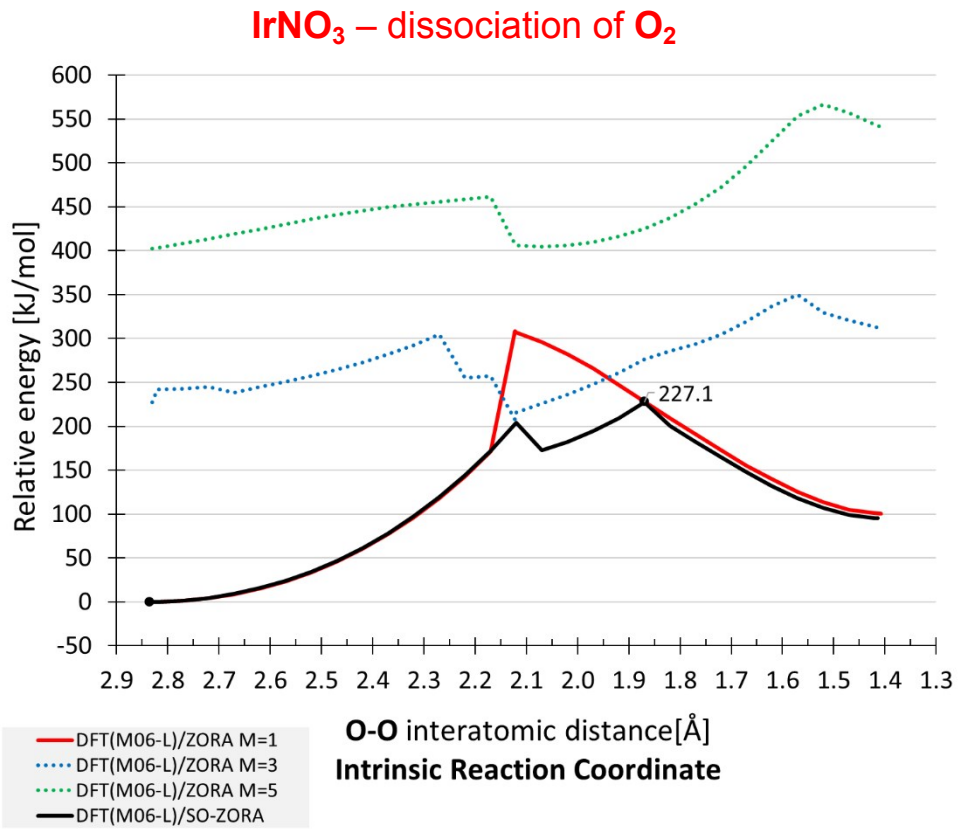


Figure S29. Reaction of **O_2 ligand** dissociation from **$IrNO_3$** molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown. This data for $IrNO_3$ we quote for our previous work [1].

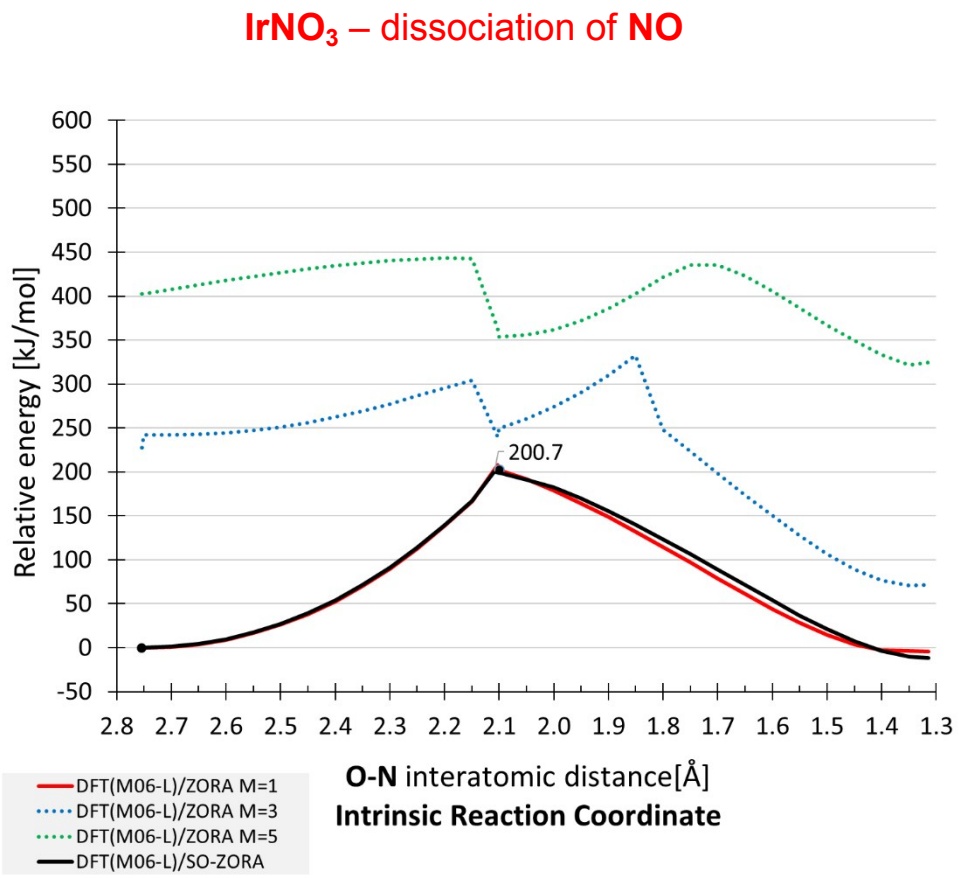


Figure S30. Reaction of **O_2 ligands** dissociation from **$IrNO_3$** molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown. This data for $IrNO_3$ we quote for our previous work [1].

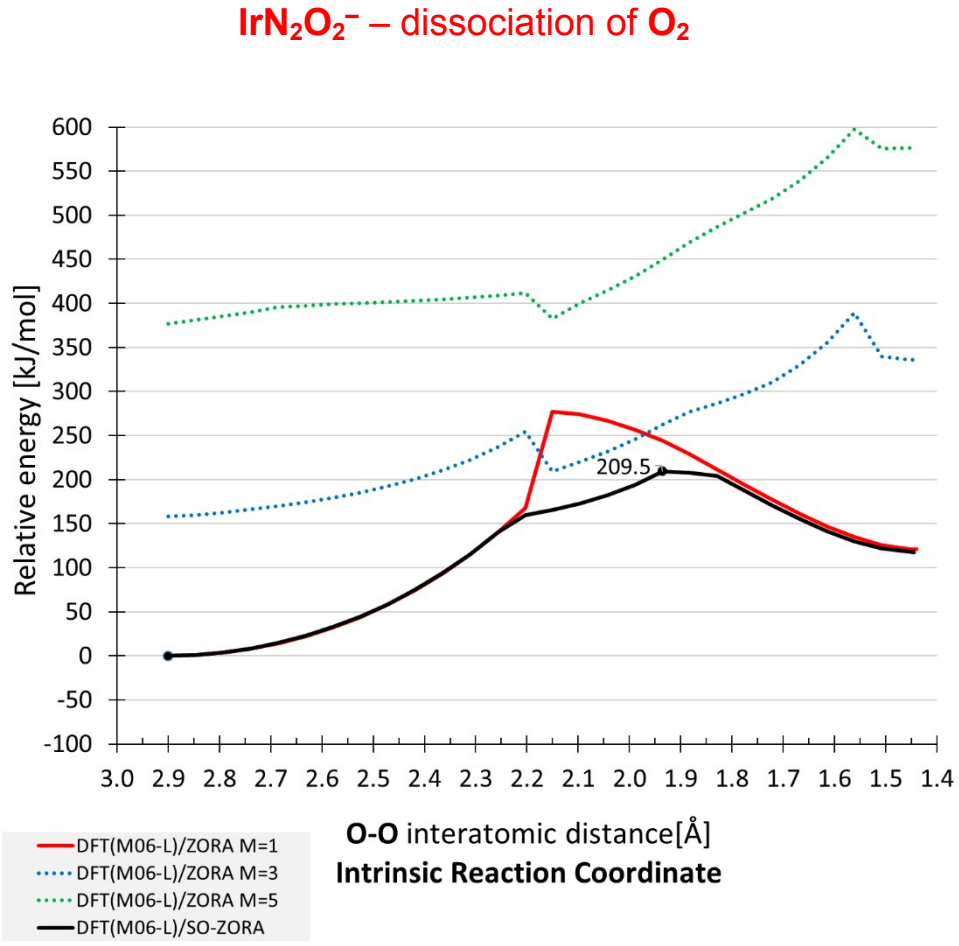
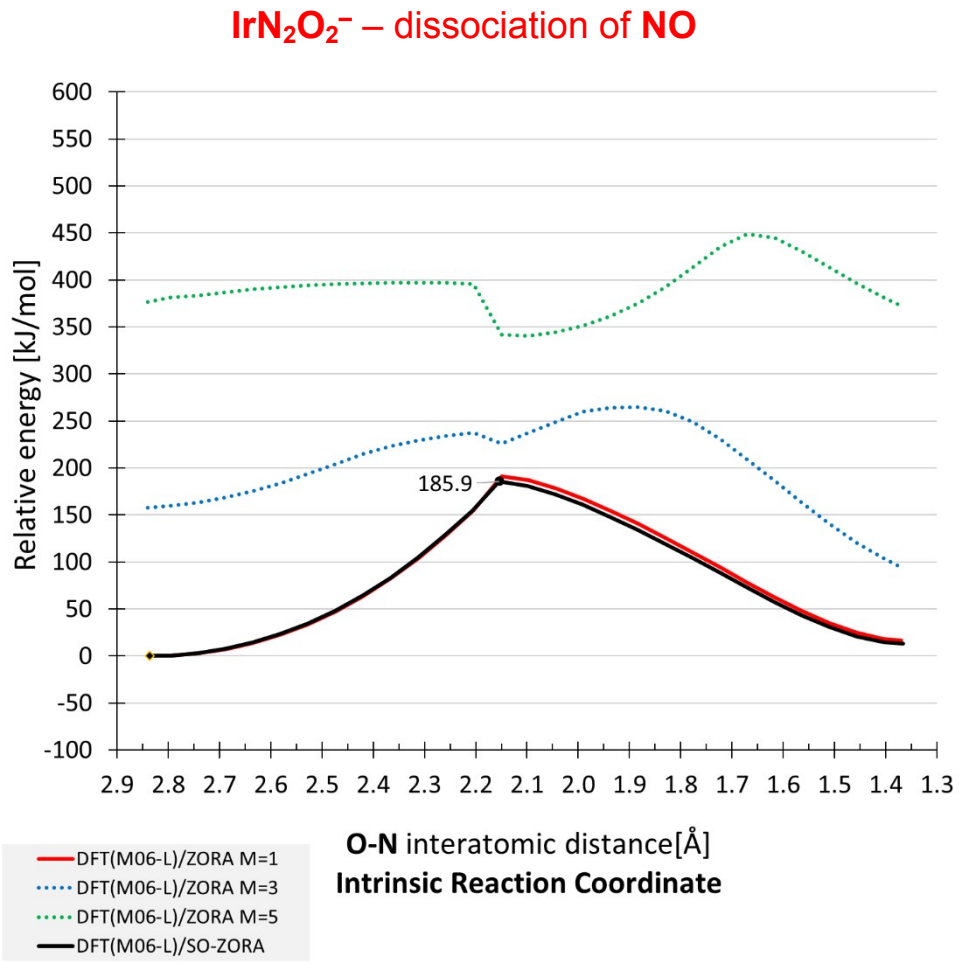
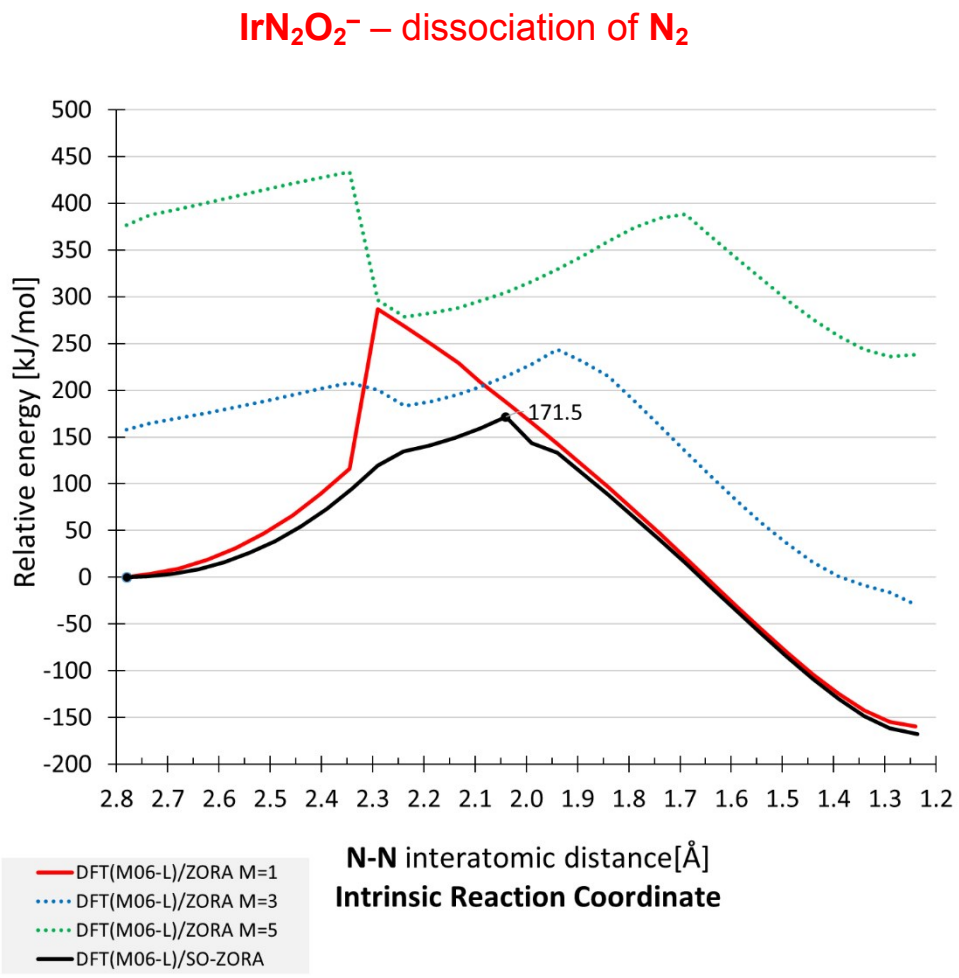


Figure S31. Reaction of **O_2 ligand** dissociation from **$IrN_2O_2^-$** anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.



Figures S32. Reaction of **NO ligand** dissociation from $IrN_2O_2^-$ anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.



Figures S33. Reaction of **N_2 ligand** dissociation from **$IrN_2O_2^-$** anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

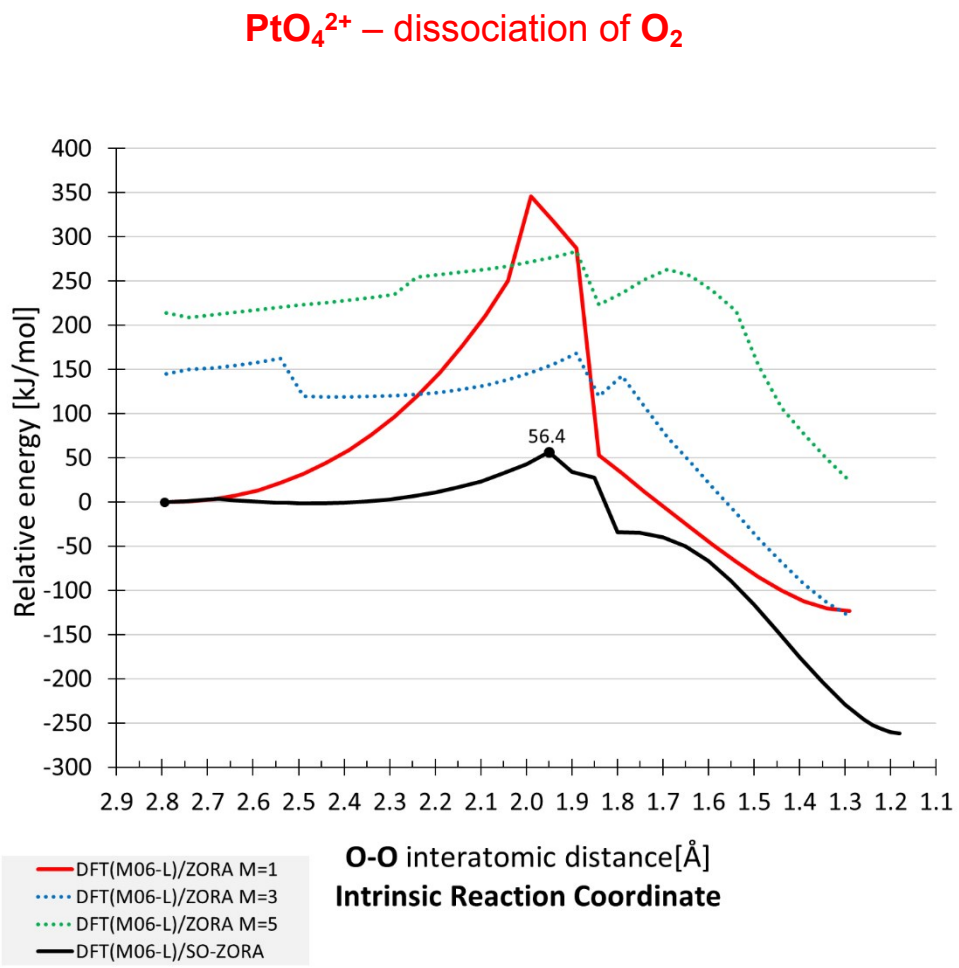


Figure S34. Reaction of **O_2 ligand** dissociation from **PtO_4^{2+}** dication. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

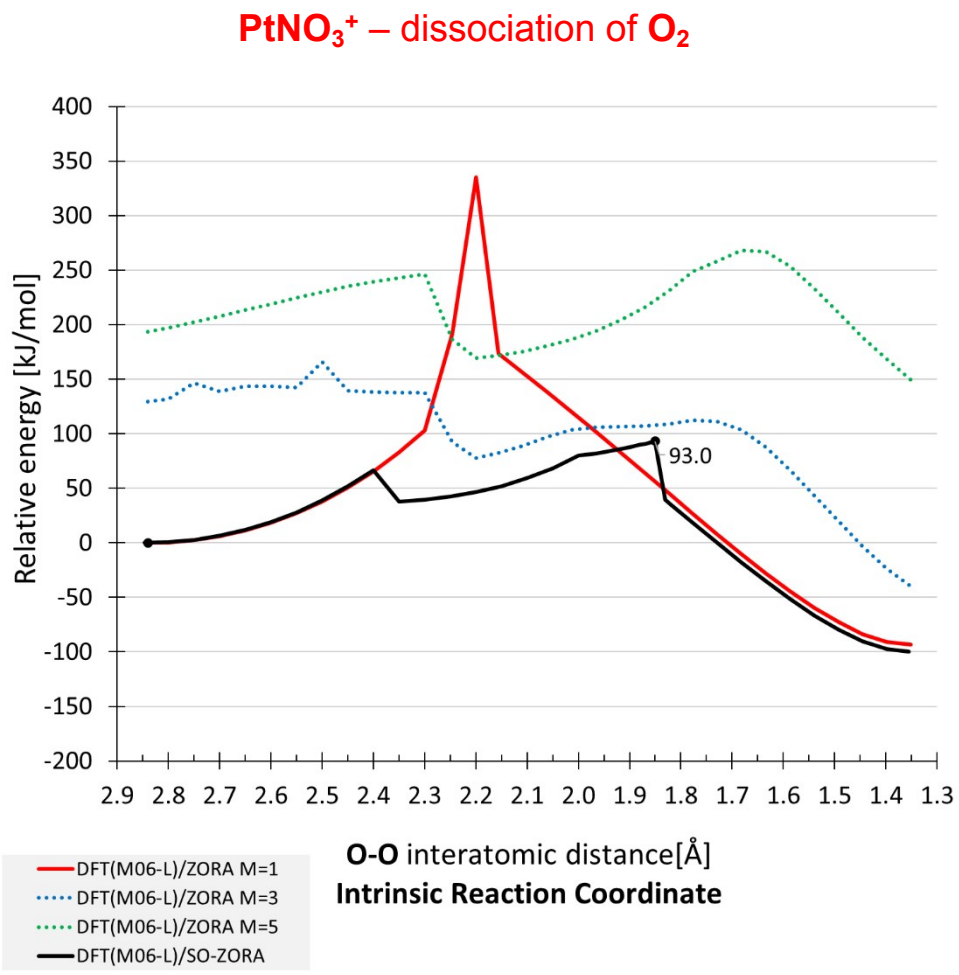


Figure S35. Reaction of **O_2 ligand** dissociation from **$PtNO_3^+$** cation. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

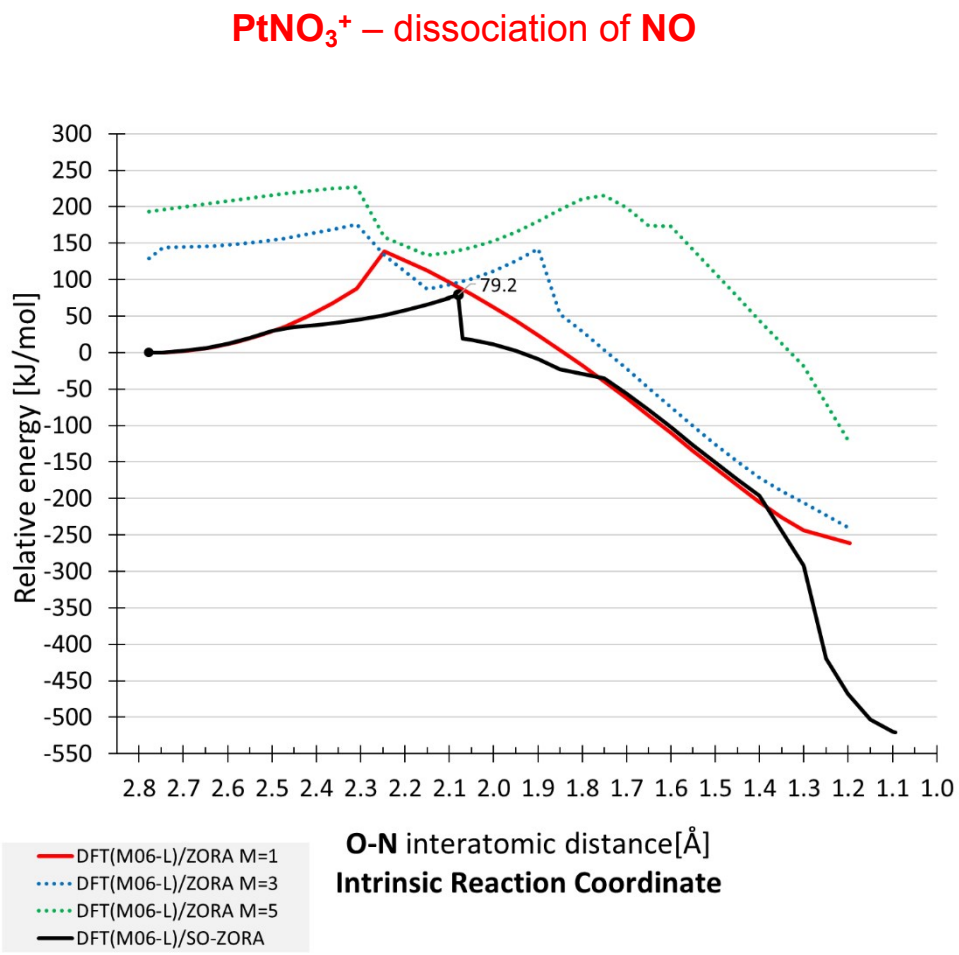


Figure S36. Reaction of **NO ligand** dissociation from **$PtNO_3^+$** cation Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

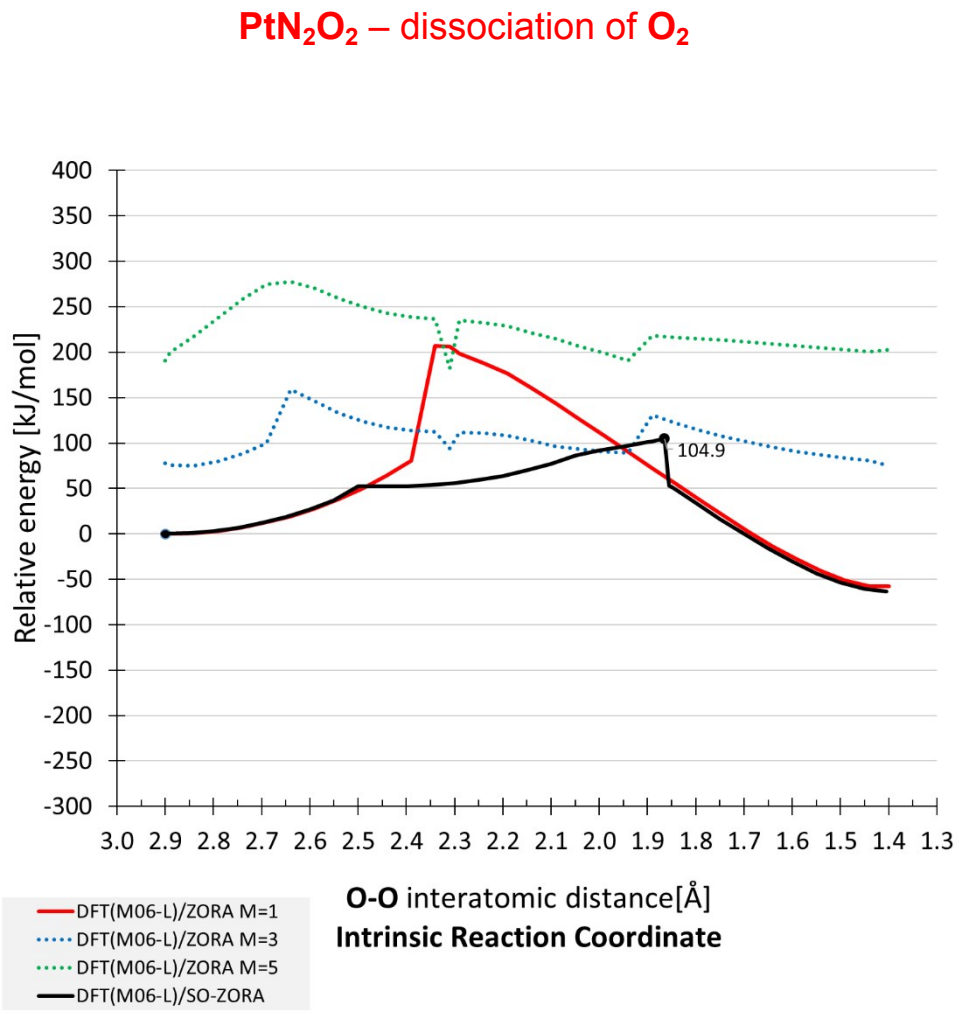


Figure S37. Reaction of **O_2 ligand** dissociation from **PtN_2O_2** molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

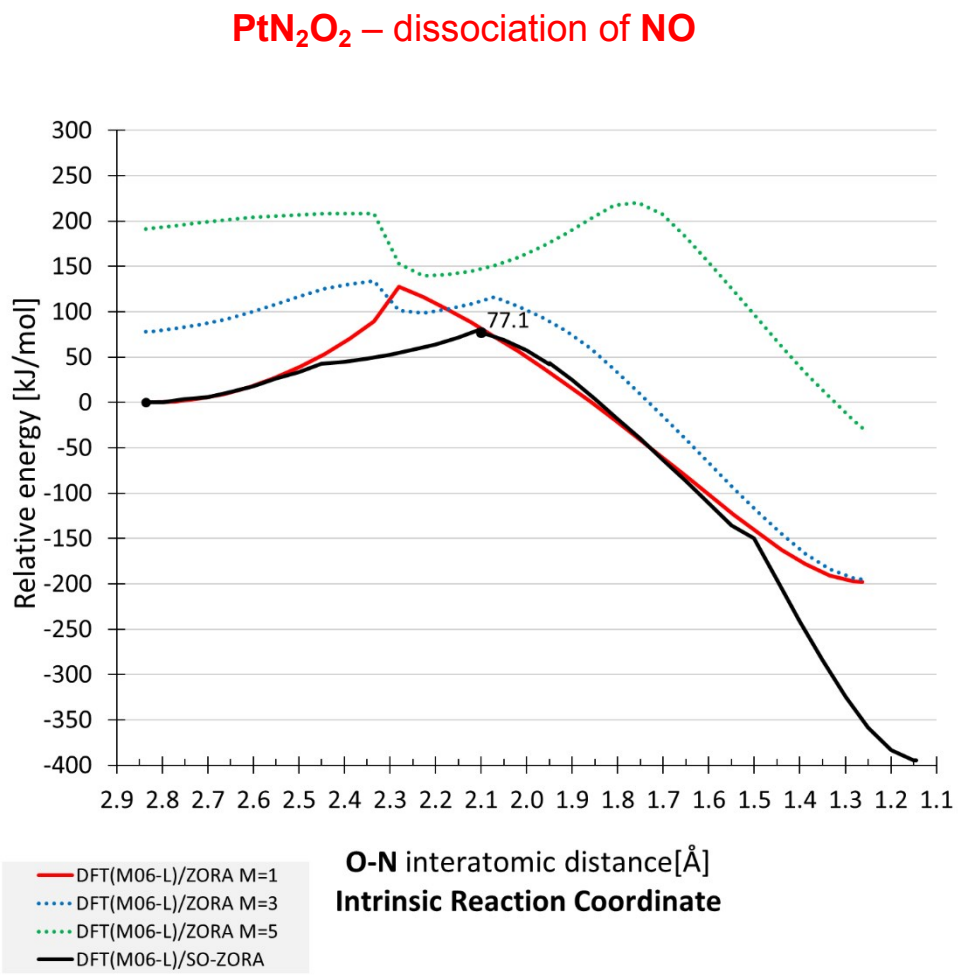


Figure S38. Reaction of **NO ligand** dissociation from **PtN_2O_2** molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

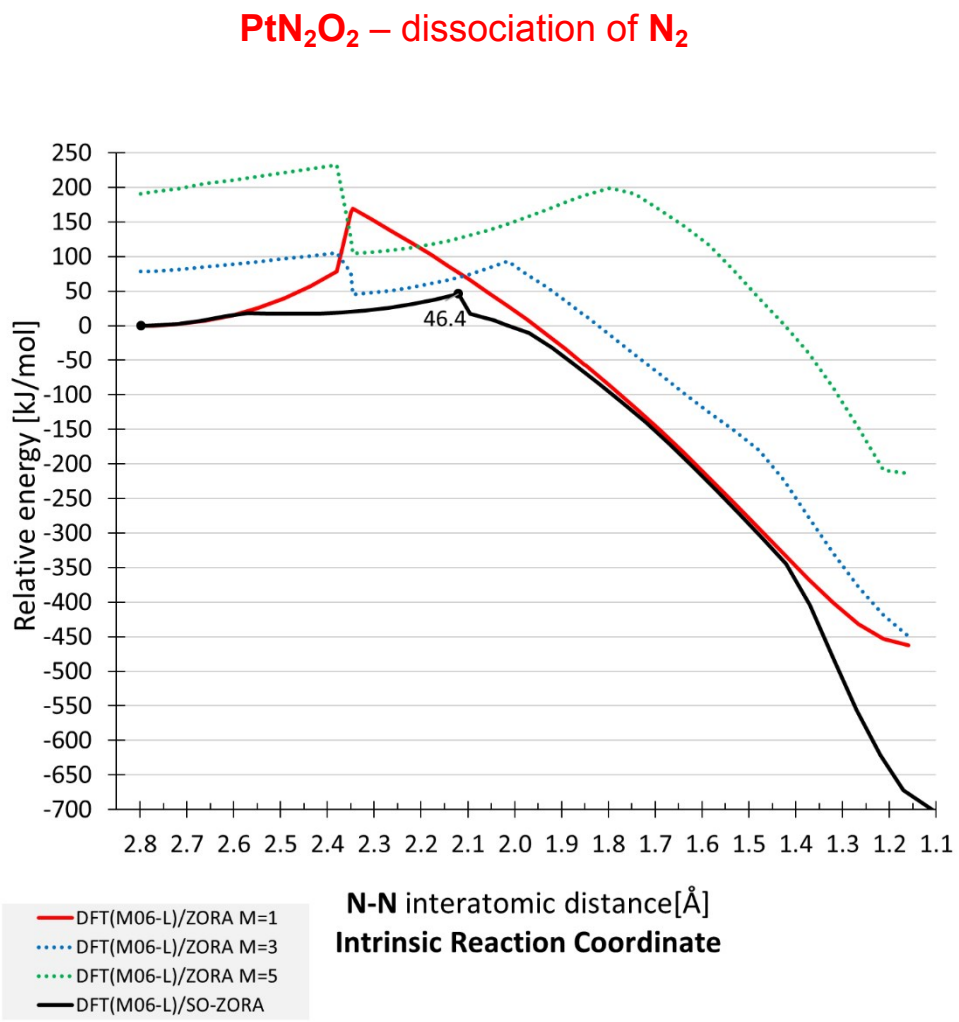


Figure S39. Reaction of **N_2 ligand** dissociation from **PtN_2O_2** molecule. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

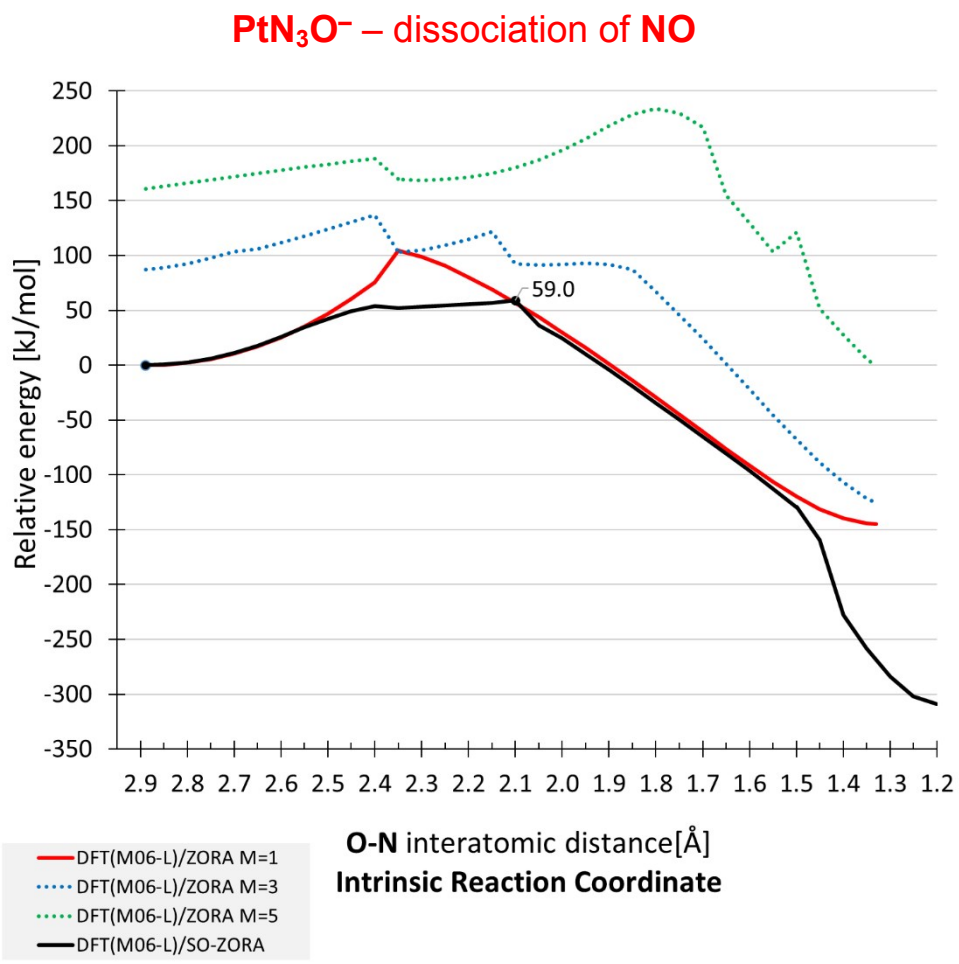


Figure S40. Reaction of **NO ligand** dissociation from **PtN_3O^-** anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

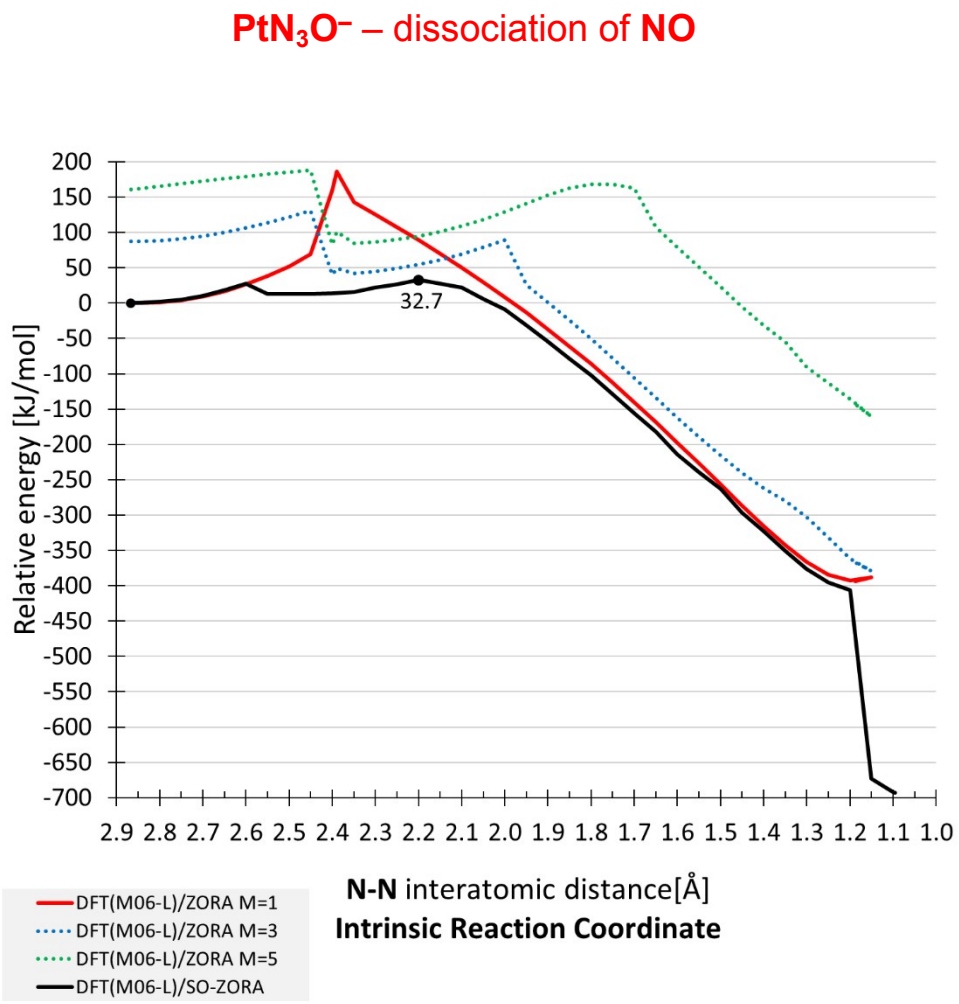


Figure S41. Reaction of **NO ligand** dissociation from **PtN_3O^-** anion. Reaction path leads from minimum structure (most left) with the metal atom at the highest formal oxidation state. As all shown energies ale relative, energy of this structure is set to zero (black dot). Reaction path was obtained with DFT/SO-ZORA approach by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance and allowing all others to optimize. DFT/SO-ZORA dissociation energy barrier is labelled. For comparison purposes singlet electron multiplicity (M=1) path (geometries were optimized with an arbitrary constraint on chosen interatomic distance) computed at DFT/ZORA level of theory with corresponding vertical energy curves for triplet (M=3) and quintet (M=5) multiplicities (single-point energies for equilibrium geometries for M=1) are shown.

Table S1. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **OsO_4** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown.

OsO_4 – dissociation of O_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓		O-O interatomic distance ↓ [Å]	Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.773**	**-18108.34907**	**-18108.21046**	**-18108.08400**	**0.0**	**363.9**	**696.0**	**-18104.56381**	**0.0**	**0.016**
2		2.740	-18108.34893	-18108.20367	-18108.08301	0.4	381.7	698.5	-18104.56377	0.1	0.016
3		2.690	-18108.34812	-18108.20331	-18108.08160	2.5	382.7	702.3	-18104.56365	0.4	0.016
4		2.640	-18108.34656	-18108.20260	-18108.08033	6.6	384.6	705.6	-18104.56282	2.6	0.016
5		2.590	-18108.34426	-18108.20151	-18108.07924	12.6	387.4	708.5	-18104.56128	6.6	0.016
6		2.540	-18108.34116	-18108.20001	-18108.07836	20.8	391.4	710.8	-18104.55900	12.6	0.016
7		2.490	-18108.33725	-18108.19812	-18108.07773	31.0	396.3	712.4	-18104.55595	20.6	0.016
8		2.440	-18108.33249	-18108.19582	-18108.07736	43.6	402.4	713.4	-18104.55211	30.7	0.016
9		2.390	-18108.32681	-18108.20835	-18108.07721	58.5	369.5	713.8	-18104.54742	43.0	0.016
10		2.340	-18108.32016	-18108.20902	-18108.07722	75.9	367.7	713.8	-18104.54185	57.7	0.016
11		2.290	-18108.31247	-18108.20962	-18108.07729	96.1	366.1	713.6	-18104.53532	74.8	0.016
12		2.240	-18108.30365	-18108.21005	-18108.07735	119.3	365.0	713.4	-18104.52777	94.6	0.016
13		2.190	-18108.29358	-18108.21021	-18108.07730	145.7	364.6	713.5	-18104.51912	117.3	0.016
14		2.140	-18108.28215	-18108.20997	-18108.07698	175.7	365.2	714.4	-18104.50926	143.2	0.016
15		2.090	-18108.26921	-18108.20921	-18108.07624	209.7	367.2	716.3	-18104.49808	172.6	0.016
16		2.040	-18108.25458	-18108.20777	-18108.07488	248.1	371.0	719.9	-18104.48546	205.7	0.017
17	**B**	**1.986**	**-18108.19431**	**-18108.22171**	**-18108.12685**	**406.3**	**334.4**	**583.5**	**-18104.41567**	**388.9**	**0.029**
18		1.940	-18108.18817	-18108.21358	-18108.13641	422.5	355.7	558.3	-18104.47124	243.0	0.017
19		1.890	-18108.19575	-18108.20818	-18108.13416	402.6	369.9	564.3	-18104.42197	372.4	0.020
20		1.840	-18108.20322	-18108.20147	-18108.13087	382.9	387.5	572.9	-18104.42643	360.7	0.019
21		1.790	-18108.21051	-18108.19328	-18108.12638	363.8	409.0	584.7	-18104.43138	347.7	0.019
22		1.740	-18108.21758	-18108.18343	-18108.12046	345.2	434.9	600.2	-18104.43660	334.0	0.019
23		1.690	-18108.22433	-18108.17184	-18108.11285	327.5	465.3	620.2	-18104.44199	319.8	0.018
24		1.640	-18108.23058	-18108.15889	-18108.10326	311.1	499.3	645.4	-18104.44740	305.6	0.018
25		1.590	-18108.23615	-18108.17355	-18108.09164	296.5	460.8	675.9	-18104.45266	291.8	0.018
26		1.540	-18108.24084	-18108.17670	-18108.07857	284.2	452.6	710.2	-18104.45757	278.9	0.018
27		1.490	-18108.24431	-18108.17871	-18108.06715	275.1	447.3	740.2	-18104.46190	267.5	0.018
28		1.440	-18108.24612	-18108.17912	-18108.06280	270.3	446.2	751.6	-18104.46537	258.5	0.018
29	**C**	**1.421**	**-18108.24627**	**-18108.17870**	**-18108.06305**	**269.9**	**447.3**	**750.9**	**-18104.46788**	**251.9**	**0.018**

Table S2. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **$OsNO_3^-$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown.

$OsNO_3^-$ – dissociation of O_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓		O-O interatomic distance ↓ [Å]	Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.864**	**-18087.89660**	**-18087.77823**	**-18087.67150**	**0.0**	**310.8**	**591.0**	**-18084.13994**	**0.0**	**0.015**
2		2.840	-18087.89653	-18087.77340	-18087.67070	0.2	323.4	593.1	-18084.13986	0.2	0.015
3		2.790	-18087.89592	-18087.77321	-18087.66886	1.8	324.0	597.9	-18084.13923	1.9	0.015
4		2.740	-18087.89469	-18087.77590	-18087.66698	5.0	316.9	602.9	-18084.13800	5.1	0.015
5		2.690	-18087.89283	-18087.77366	-18087.66510	9.9	322.8	607.8	-18084.13614	10.0	0.015
6		2.640	-18087.89031	-18087.77198	-18087.66328	16.5	327.2	612.6	-18084.13364	16.5	0.015
7		2.590	-18087.88712	-18087.77020	-18087.66156	24.9	331.9	617.1	-18084.13047	24.9	0.016
8		2.540	-18087.88324	-18087.76829	-18087.65999	35.1	336.9	621.2	-18084.12662	35.0	0.016
9		2.490	-18087.87862	-18087.76621	-18087.65861	47.2	342.3	624.8	-18084.12204	47.0	0.016
10		2.440	-18087.87323	-18087.76388	-18087.65749	61.3	348.4	627.8	-18084.11671	61.0	0.016
11		2.390	-18087.86702	-18087.76117	-18087.65666	77.7	355.6	629.9	-18084.11056	77.1	0.016
12		2.340	-18087.85992	-18087.75793	-18087.65610	96.3	364.1	631.4	-18084.10354	95.6	0.017
13		2.290	-18087.85187	-18087.76515	-18087.65572	117.4	345.1	632.4	-18084.09558	116.5	0.017
14		2.240	-18087.84278	-18087.76468	-18087.65539	141.3	346.4	633.3	-18084.08661	140.0	0.017
15		2.190	-18087.83254	-18087.76406	-18087.65497	168.2	348.0	634.4	-18084.07652	166.5	0.018
16		2.140	-18087.82103	-18087.76316	-18087.65431	198.4	350.3	636.1	-18084.06521	196.2	0.018
17		2.090	-18087.80811	-18087.76183	-18087.65324	232.3	353.8	638.9	-18084.05256	229.4	0.019
18		2.040	-18087.79364	-18087.75989	-18087.65154	270.3	358.9	643.4	-18084.03843	266.5	0.019
19		1.990	-18087.75238	-18087.77065	-18087.66802	378.6	330.7	600.1	-18084.00218	361.7	0.028
20	**B**	**1.987**	**-18087.75237**	**-18087.77013**	**-18087.66763**	**378.7**	**332.0**	**601.2**	**-18084.00241**	**361.1**	**0.028**
21		1.940	-18087.75324	-18087.76349	-18087.66612	376.4	349.5	605.1	-18084.00596	351.8	0.026
22		1.890	-18087.75552	-18087.75638	-18087.66539	370.4	368.1	607.0	-18084.01034	340.3	0.024
23		1.840	-18087.75884	-18087.74860	-18087.66373	361.7	388.6	611.4	-18084.01558	326.5	0.022
24		1.790	-18087.76320	-18087.73998	-18087.66096	350.2	411.2	618.7	-18084.02167	310.5	0.020
25		1.740	-18087.76877	-18087.73108	-18087.65707	335.6	434.6	628.9	-18084.02855	292.5	0.019
26		1.690	-18087.77487	-18087.72091	-18087.64925	319.6	461.3	649.4	-18084.03375	278.8	0.018
27		1.640	-18087.78045	-18087.71417	-18087.63910	304.9	479.0	676.0	-18084.03838	266.6	0.018
28		1.590	-18087.78535	-18087.69661	-18087.62651	292.1	525.1	709.1	-18084.04239	256.1	0.018
29		1.540	-18087.78934	-18087.68420	-18087.61115	281.6	557.6	749.4	-18084.04548	248.0	0.018
30		1.490	-18087.79209	-18087.71379	-18087.59321	274.4	480.0	796.5	-18084.04729	243.2	0.018
31		1.440	-18087.79311	-18087.71286	-18087.58581	271.7	482.4	816.0	-18084.04737	243.0	0.018
32	**C**	**1.439**	**-18087.79312**	**-18087.71271**	**-18087.58585**	**271.7**	**482.8**	**815.9**	**-18084.04737**	**243.0**	**0.018**

Table S3. Potential energy characteristics of reaction-path of **dissociation of NO ligand** from the **$OsNO_3^-$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B'** to other minimum energy structure **C'** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown.

$OsNO_3^-$ – dissociation of NO

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-O interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.784**	**-18087.89660**	**-18087.77823**	**-18087.67150**	**0.0**	**310.8**	**591.0**	**-18084.13994**	**0.0**	**0.015**
2		2.770	-18087.89659	-18087.77338	-18087.67095	0.0	323.5	592.4	-18084.13994	0.0	0.015
3		2.720	-18087.89610	-18087.77332	-18087.66880	1.3	323.7	598.1	-18084.13949	1.2	0.015
4		2.670	-18087.89484	-18087.77289	-18087.66670	4.6	324.8	603.6	-18084.13831	4.3	0.015
5		2.620	-18087.89279	-18087.77209	-18087.66470	10.0	326.9	608.8	-18084.13637	9.4	0.015
6		2.570	-18087.88993	-18087.77090	-18087.66286	17.5	330.0	613.7	-18084.13366	16.5	0.015
7		2.520	-18087.88623	-18087.76933	-18087.66125	27.2	334.1	617.9	-18084.13014	25.7	0.015
8		2.470	-18087.88165	-18087.76737	-18087.65991	39.2	339.3	621.4	-18084.12580	37.1	0.016
9		2.420	-18087.87617	-18087.76500	-18087.65885	53.6	345.5	624.2	-18084.12059	50.8	0.016
10		2.370	-18087.86972	-18087.76639	-18087.65808	70.6	341.9	626.2	-18084.11448	66.8	0.016
11		2.320	-18087.86226	-18087.76566	-18087.65756	90.1	343.8	627.6	-18084.10743	85.3	0.016
12		2.270	-18087.85375	-18087.76492	-18087.65724	112.5	345.7	628.4	-18084.09943	106.4	0.017
13		2.220	-18087.84414	-18087.76410	-18087.65711	137.7	347.9	628.8	-18084.09045	129.9	0.018
14		2.170	-18087.83339	-18087.76309	-18087.65716	166.0	350.5	628.6	-18084.08052	156.0	0.020
15		2.120	-18087.82151	-18087.76184	-18087.65751	197.1	353.8	627.7	-18084.06974	184.3	0.023
16		2.070	-18087.80863	-18087.76052	-18087.65876	230.9	357.3	624.4	-18084.05841	214.1	0.027
17		2.020	-18087.79526	-18087.75982	-18087.66357	266.0	359.1	611.8	-18084.04722	243.4	0.031
18	**B'**	**1.972**	**-18087.78966**	**-18087.75897**	**-18087.69182**	**280.7**	**361.3**	**537.6**	**-18084.03713**	**269.9**	**0.027**
19		1.970	-18087.78966	-18087.75870	-18087.69189	280.8	362.0	537.5	-18084.03707	270.1	0.027
20		1.920	-18087.79063	-18087.75187	-18087.69188	278.2	380.0	537.5	-18084.03812	267.3	0.026
21		1.870	-18087.79311	-18087.74323	-18087.68984	271.7	402.7	542.8	-18084.04140	258.7	0.025
22		1.820	-18087.79658	-18087.74367	-18087.68633	262.6	401.5	552.0	-18084.04554	247.9	0.024
23		1.770	-18087.80077	-18087.74510	-18087.68124	251.6	397.8	565.4	-18084.05005	236.0	0.023
24		1.720	-18087.80544	-18087.74719	-18087.67473	239.3	392.3	582.5	-18084.05470	223.8	0.023
25		1.670	-18087.81034	-18087.74963	-18087.66775	226.5	385.9	600.8	-18084.05932	211.7	0.023
26		1.620	-18087.81524	-18087.75211	-18087.66257	213.6	379.3	614.4	-18084.06375	200.0	0.023
27		1.570	-18087.81985	-18087.74825	-18087.66182	201.5	389.5	616.4	-18084.06782	189.3	0.023
28		1.520	-18087.82388	-18087.75616	-18087.66490	190.9	368.7	608.3	-18084.07130	180.2	0.023
29		1.470	-18087.82697	-18087.76331	-18087.66928	182.8	349.9	596.8	-18084.07393	173.3	0.023
30		1.420	-18087.82871	-18087.76931	-18087.67351	178.2	334.2	585.7	-18084.07534	169.6	0.024
31	**C'**	**1.396**	**-18087.82892**	**-18087.77157**	**-18087.67513**	**177.7**	**328.3**	**581.5**	**-18084.07545**	**169.3**	**0.024**

Table S4. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **IrO_4^+** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

IrO_4^+ – dissociation of O_2

No of step on the pathway ↓		O-O interatomic distance ↓ [Å]	DFT(M06-L)/ZORA						CCSD(T)/ZORA		
			Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.755**	**-18716.57834**	**-18716.48179**	**-18716.40277**	**0.0**	**253.5**	**461.0**	**-18712.74981**	**0.0**	**0.017**
2		2.720	-18716.57819	-18716.47441	-18716.40185	0.4	272.9	463.4	-18712.74946	0.9	0.017
3		2.670	-18716.57735	-18716.47392	-18716.40054	2.6	274.2	466.8	-18712.74837	3.8	0.017
4		2.620	-18716.57575	-18716.47306	-18716.39928	6.8	276.4	470.1	-18712.74659	8.5	0.017
5		2.570	-18716.57337	-18716.47182	-18716.39810	13.1	279.7	473.2	-18712.74408	15.1	0.017
6		2.520	-18716.57017	-18716.48042	-18716.39704	21.5	257.1	476.0	-18712.74080	23.6	0.017
7		2.470	-18716.56611	-18716.48056	-18716.39610	32.1	256.7	478.5	-18712.73673	34.3	0.017
8		2.420	-18716.56114	-18716.48077	-18716.39528	45.2	256.2	480.6	-18712.73180	47.3	0.017
9		2.370	-18716.55521	-18716.48099	-18716.39452	60.7	255.6	482.6	-18712.72597	62.6	0.017
10		2.320	-18716.54824	-18716.48115	-18716.39383	79.0	255.2	484.4	-18712.71917	80.4	0.017
11		2.270	-18716.54015	-18716.48116	-18716.39312	100.3	255.2	486.3	-18712.71132	101.1	0.017
12		2.220	-18716.53083	-18716.48093	-18716.39230	124.7	255.8	488.5	-18712.70233	124.7	0.018
13		2.170	-18716.50545	-18716.50292	-18716.42217	191.4	198.0	410.0	-18712.68440	171.7	0.046
14	**B**	**2.123**	**-18716.45810**	**-18716.49858**	**-18716.43664**	**315.7**	**209.4**	**372.0**	**-18712.65455**	**250.1**	**0.047**
15		2.070	-18716.40095	-18716.49599	-18716.44078	311.0	216.2	361.2	-18712.65787	241.4	0.023
16		2.020	-18716.46552	-18716.49264	-18716.43958	296.2	225.0	364.3	-18712.66102	233.1	0.023
17		1.970	-18716.47314	-18716.48841	-18716.43782	276.2	236.1	368.9	-18712.66500	222.7	0.022
18		1.920	-18716.48084	-18716.48304	-18716.43512	256.0	250.2	376.0	-18712.66950	210.8	0.022
19		1.870	-18716.48856	-18716.47655	-18716.43167	235.7	267.3	385.1	-18712.67443	197.9	0.022
20		1.820	-18716.49621	-18716.46864	-18716.42699	215.6	288.0	397.4	-18712.67969	184.1	0.021
21		1.770	-18716.50375	-18716.45936	-18716.42127	195.8	312.4	412.4	-18712.68514	169.8	0.021
22		1.720	-18716.51113	-18716.44846	-18716.41406	176.5	341.0	431.3	-18712.69067	155.3	0.021
23		1.670	-18716.51824	-18716.43649	-18716.40577	157.8	372.4	453.1	-18712.69609	141.0	0.021
24		1.620	-18716.52491	-18716.45848	-18716.39699	140.3	314.7	476.1	-18712.70123	127.5	0.021
25		1.570	-18716.53099	-18716.46252	-18716.39148	124.3	304.1	490.6	-18712.70586	115.4	0.021
26		1.520	-18716.53627	-18716.46603	-18716.39263	110.5	294.9	487.6	-18712.70971	105.3	0.022
27		1.470	-18716.54043	-18716.46824	-18716.39790	99.5	289.1	473.7	-18712.71249	98.0	0.022
28		1.420	-18716.54305	-18716.47961	-18716.40400	92.7	259.2	457.7	-18712.71379	94.6	0.023
29	**C**	**1.380**	**-18716.54371**	**-18716.48522**	**-18716.40826**	**90.9**	**244.5**	**446.6**	**-18712.71345**	**95.5**	**0.024**

Table S5. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **$IrNO_3$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red). All data for $IrNO_3$ we quote for our previous work [1].

$IrNO_3$ – dissociation of O_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓		O-O interatomic distance ↓ [Å]	Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.830**	**-18696.40616**	**-18696.31945**	**-18696.25294**	**0.0**	**227.6**	**402.3**	**-18692.60329**	**0.0**	**0.020**
2		2.820	-18696.40615	-18696.31391	-18696.25257	0.0	242.2	403.2	-18692.60325	0.1	0.020
3		2.770	-18696.40570	-18696.31367	-18696.25068	1.2	242.8	408.2	-18692.60267	1.6	0.020
4		2.720	-18696.40461	-18696.31287	-18696.24866	4.1	244.9	413.5	-18692.60149	4.7	0.020
5		2.670	-18696.40286	-18696.31540	-18696.24656	8.7	238.3	419.0	-18692.59968	9.5	0.021
6		2.620	-18696.40042	-18696.31282	-18696.24442	15.1	245.1	424.7	-18692.59723	15.9	0.021
7		2.570	-18696.39727	-18696.31058	-18696.24227	23.3	250.9	430.3	-18692.59410	24.1	0.022
8		2.520	-18696.39338	-18696.30812	-18696.24018	33.5	257.4	435.8	-18692.59026	34.2	0.023
9		2.470	-18696.38872	-18696.30539	-18696.23821	45.8	264.6	440.9	-18692.58568	46.2	0.024
10		2.420	-18696.38323	-18696.30233	-18696.23642	60.2	272.6	445.7	-18692.58031	60.4	0.024
11		2.370	-18696.37685	-18696.29885	-18696.23488	76.9	281.7	449.7	-18692.57408	76.7	0.025
12		2.320	-18696.36952	-18696.29481	-18696.23363	96.2	292.4	453.0	-18692.56696	95.4	0.026
13		2.270	-18696.36115	-18696.29009	-18696.23259	118.2	304.7	455.7	-18692.55885	116.7	0.026
14		2.220	-18696.35167	-18696.30885	-18696.23160	143.1	255.5	458.3	-18692.54967	140.8	0.027
15		2.170	-18696.34095	-18696.30820	-18696.23050	171.2	257.2	461.2	-18692.53935	167.9	0.028
16	**B**	**2.122**	**-18696.28865**	**-18696.32706**	**-18696.25095**	**308.5**	**207.7**	**407.5**	**-18692.52208**	**213.2**	**0.055**
17		2.120	-18696.28939	-18696.32398	-18696.25159	306.6	215.8	405.8	-18692.50936	246.6	0.034
18		2.070	-18696.29353	-18696.32004	-18696.25200	295.7	226.1	404.7	-18692.51478	232.4	0.032
19		2.020	-18696.29875	-18696.31617	-18696.25142	282.0	236.3	406.3	-18692.51956	219.8	0.029
20		1.970	-18696.30490	-18696.31185	-18696.25001	265.9	247.6	410.0	-18692.52472	206.3	0.026
21		1.920	-18696.31193	-18696.30670	-18696.24772	247.4	261.1	416.0	-18692.53030	191.7	0.023
22		1.870	-18696.31923	-18696.30102	-18696.24415	228.2	276.0	425.4	-18692.53540	178.2	0.023
23		1.820	-18696.32643	-18696.29732	-18696.23950	209.3	285.8	437.6	-18692.54076	164.2	0.022
24		1.770	-18696.33348	-18696.29415	-18696.23357	190.8	294.1	453.1	-18692.54626	149.7	0.022
25		1.720	-18696.34036	-18696.29011	-18696.22617	172.8	304.7	472.5	-18692.55176	135.3	0.022
26		1.670	-18696.34692	-18696.28454	-18696.21707	155.5	319.3	496.5	-18692.55709	121.3	0.022
27		1.620	-18696.35299	-18696.27796	-18696.20631	139.6	336.6	524.7	-18692.56207	108.2	0.022
28		1.570	-18696.35840	-18696.27276	-18696.19541	125.4	350.2	553.3	-18692.56644	96.7	0.022
29		1.520	-18696.36292	-18696.28060	-18696.19036	113.5	329.6	566.6	-18692.56993	87.6	0.022
30		1.470	-18696.36618	-18696.28388	-18696.19395	105.0	321.0	557.2	-18692.57216	81.8	0.022
31		1.420	-18696.36773	-18696.28685	-18696.19900	100.9	313.2	543.9	-18692.57267	80.4	0.022
32	**C**	**1.408**	**-18696.36779**	**-18696.28753**	**-18696.20014**	**100.7**	**311.5**	**540.9**	**-18692.57249**	**80.9**	**0.022**

Table S6. Potential energy characteristics of reaction-path of **dissociation of NO** ligand from the **$IrNO_3$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B'** to other minimum energy structure **C'** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red). All data for $IrNO_3$ we quote for our previous work [1].

$IrNO_3$ – dissociation of **NO**

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-O interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	A	2.754	-18696.40616	-18696.31945	-18696.25294	0.0	227.6	402.3	-18692.60329	0.0	0.020
2		2.750	-18696.40616	-18696.31395	-18696.25284	0.0	242.1	402.5	-18692.60329	0.0	0.020
3		2.700	-18696.40580	-18696.31405	-18696.25094	0.9	241.8	407.5	-18692.60279	1.3	0.020
4		2.650	-18696.40465	-18696.31376	-18696.24902	3.9	242.6	412.6	-18692.60156	4.5	0.020
5		2.600	-18696.40269	-18696.31308	-18696.24711	9.1	244.4	417.6	-18692.59958	9.7	0.021
6		2.550	-18696.39988	-18696.31199	-18696.24526	16.5	247.2	422.4	-18692.59683	17.0	0.021
7		2.500	-18696.39619	-18696.31050	-18696.24354	26.2	251.2	426.9	-18692.59327	26.3	0.022
8		2.450	-18696.39160	-18696.30859	-18696.24199	38.2	256.2	431.0	-18692.58889	37.8	0.023
9		2.400	-18696.38605	-18696.30628	-18696.24063	52.8	262.2	434.6	-18692.58366	51.5	0.025
10		2.350	-18696.37949	-18696.30356	-18696.23947	70.0	269.4	437.6	-18692.57758	67.5	0.027
11		2.300	-18696.37190	-18696.30047	-18696.23851	89.9	277.5	440.1	-18692.57063	85.7	0.030
12		2.250	-18696.36324	-18696.29709	-18696.23779	112.7	286.4	442.1	-18692.56283	106.2	0.032
13		2.200	-18696.35349	-18696.29358	-18696.23736	138.3	295.6	443.2	-18692.55422	128.8	0.035
14		2.150	-18696.34273	-18696.29034	-18696.23752	166.5	304.1	442.8	-18692.54486	153.4	0.038
15	**B'**	**2.103**	**-18696.32699**	**-18696.31476**	**-18696.26783**	**207.8**	**240.0**	**363.2**	**-18692.52975**	**193.1**	**0.033**
16		2.100	-18696.32919	-18696.31110	-18696.27151	202.1	249.6	353.5	-18692.53183	187.6	0.034
17		2.050	-18696.33314	-18696.30688	-18696.27064	191.7	260.7	355.8	-18692.53790	171.7	0.034
18		2.000	-18696.33801	-18696.30177	-18696.26826	178.9	274.1	362.0	-18692.54414	155.3	0.033
19		1.950	-18696.34352	-18696.29555	-18696.26441	164.5	290.4	372.2	-18692.55266	132.9	0.034
20		1.900	-18696.34951	-18696.28813	-18696.25914	148.7	309.9	386.0	-18692.55579	124.7	0.030
21		1.850	-18696.35585	-18696.27955	-18696.25269	132.1	332.4	402.9	-18692.56151	109.7	0.028
22		1.800	-18696.36247	-18696.31183	-18696.24561	114.7	247.6	421.5	-18692.56737	94.3	0.027
23		1.750	-18696.36925	-18696.32116	-18696.24022	96.9	223.2	435.7	-18692.57337	78.6	0.026
24		1.700	-18696.37610	-18696.33057	-18696.24038	78.9	198.4	435.2	-18692.57945	62.6	0.025
25		1.650	-18696.38286	-18696.33993	-18696.24515	61.2	173.9	422.7	-18692.58549	46.7	0.023
26		1.600	-18696.38936	-18696.34905	-18696.25175	44.1	149.9	405.4	-18692.59131	31.5	0.022
27		1.550	-18696.39536	-18696.35768	-18696.25901	28.4	127.3	386.3	-18692.59671	17.3	0.020
28		1.500	-18696.40060	-18696.36553	-18696.26635	14.6	106.7	367.1	-18692.60166	4.3	0.019
29		1.450	-18696.40473	-18696.37215	-18696.27321	3.7	89.3	349.1	-18692.60704	-9.8	0.028
30		1.400	-18696.40729	-18696.37699	-18696.27924	-3.0	76.6	333.2	-18692.61227	-23.6	0.039
31		1.350	-18696.40767	-18696.37933	-18696.28366	-4.0	70.4	321.6	-18692.61544	-31.9	0.046
32	**C'**	**1.315**	**-18696.40782**	**-18696.37896**	**-18696.28251**	**-4.4**	**71.4**	**324.6**	**-18692.61485**	**-30.3**	**0.044**

Table S7. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **$IrN_2O_2^-$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown.

$IrN_2O_2^-$ – dissociation of O_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	O-O interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.900**	**-18675.96268**	**-18675.90247**	**-18675.81916**	**0.0**	**158.1**	**376.8**	**-18672.18667**	**0.0**	**0.020**
2		2.846	-18675.96230	-18675.90171	-18675.81740	1.0	160.1	381.5	-18672.18606	1.6	0.020
3		2.793	-18675.96128	-18675.90071	-18675.81574	3.7	162.7	385.8	-18672.18484	4.8	0.020
4		2.739	-18675.95960	-18675.89947	-18675.81414	8.1	166.0	390.0	-18672.18299	9.7	0.020
5		2.686	-18675.95725	-18675.89800	-18675.81196	14.3	169.8	395.7	-18672.18049	16.2	0.020
6		2.632	-18675.95419	-18675.89631	-18675.81128	22.3	174.3	397.5	-18672.17731	24.6	0.020
7		2.579	-18675.95040	-18675.89436	-18675.81070	32.3	179.4	399.0	-18672.17342	34.8	0.020
8		2.525	-18675.94584	-18675.89210	-18675.81018	44.2	185.3	400.4	-18672.16879	47.0	0.020
9		2.471	-18675.94047	-18675.88945	-18675.80970	58.3	192.3	401.7	-18672.16337	61.2	0.021
10		2.418	-18675.93422	-18675.88628	-18675.80920	74.7	200.6	403.0	-18672.15711	77.6	0.021
11		2.364	-18675.92703	-18675.88249	-18675.80864	93.6	210.6	404.5	-18672.14995	96.4	0.021
12		2.311	-18675.91881	-18675.87792	-18675.80793	115.2	222.5	406.3	-18672.14180	117.8	0.021
13		2.257	-18675.90947	-18675.87245	-18675.80701	139.7	236.9	408.7	-18672.13258	142.0	0.022
14		2.204	-18675.89887	-18675.86589	-18675.80578	167.5	254.1	411.9	-18672.12217	169.4	0.022
15	**B**	**2.150**	**-18675.85714**	**-18675.88301**	**-18675.81702**	**277.1**	**209.2**	**382.5**	**-18672.08665**	**262.6**	**0.031**
16		2.096	-18675.85843	-18675.87885	-18675.81043	273.7	220.1	399.7	-18672.09322	245.4	0.031
17		2.043	-18675.86109	-18675.87446	-18675.80481	266.7	231.6	414.5	-18672.09864	231.1	0.029
18		1.989	-18675.86482	-18675.86911	-18675.79853	256.9	245.7	431.0	-18672.10411	216.8	0.028
19		1.936	-18675.86961	-18675.86276	-18675.79153	244.4	262.3	449.4	-18672.10999	201.3	0.026
20		1.882	-18675.87545	-18675.85731	-18675.78402	229.0	276.7	469.1	-18672.11648	184.3	0.024
21		1.829	-18675.88215	-18675.85362	-18675.77728	211.4	286.3	486.8	-18672.12260	168.2	0.022
22		1.775	-18675.88883	-18675.84952	-18675.77106	193.9	297.1	503.1	-18672.12801	154.0	0.022
23		1.721	-18675.89527	-18675.84436	-18675.76499	177.0	310.6	519.1	-18672.13336	140.0	0.022
24		1.668	-18675.90132	-18675.83704	-18675.75741	161.1	329.9	539.0	-18672.13846	126.6	0.021
25		1.614	-18675.90675	-18675.82715	-18675.74738	146.9	355.9	565.3	-18672.14305	114.5	0.021
26		1.561	-18675.91134	-18675.81454	-18675.73510	134.8	389.0	597.5	-18672.14683	104.6	0.021
27		1.507	-18675.91476	-18675.83345	-18675.74331	125.8	339.3	576.0	-18672.14941	97.8	0.021
28		1.454	-18675.91649	-18675.83471	-18675.74308	121.3	336.0	576.6	-18672.15029	95.5	0.020
29	**C**	**1.440**	**-18675.91658**	**-18675.83466**	**-18675.74291**	**121.0**	**336.1**	**577.0**	**-18672.15013**	**95.9**	**0.020**

Table S8. Potential energy characteristics of reaction-path of **dissociation of NO ligand** from the $IrN_2O_2^-$ molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B'** to other minimum energy structure **C'** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown.

$IrN_2O_2^-$ – dissociation of **NO**

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-O interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.840**	**-18675.96268**	**-18675.90247**	**-18675.81916**	**0.0**	**158.1**	**376.8**	**-18672.18667**	**0.0**	**0.020**
2		2.796	-18675.96254	-18675.90182	-18675.81752	0.4	159.8	381.1	-18672.18646	0.6	0.020
3		2.742	-18675.96164	-18675.90040	-18675.81661	2.7	163.5	383.5	-18672.18553	3.0	0.021
4		2.688	-18675.95994	-18675.89842	-18675.81527	7.2	168.7	387.0	-18672.18386	7.4	0.022
5		2.635	-18675.95740	-18675.89583	-18675.81412	13.9	175.5	390.1	-18672.18143	13.8	0.023
6		2.581	-18675.95401	-18675.89265	-18675.81319	22.8	183.9	392.5	-18672.17823	22.2	0.025
7		2.527	-18675.94974	-18675.88891	-18675.81249	34.0	193.7	394.3	-18672.17422	32.7	0.027
8		2.473	-18675.94453	-18675.88479	-18675.81200	47.7	204.5	395.6	-18672.16941	45.3	0.030
9		2.419	-18675.93837	-18675.88086	-18675.81167	63.8	214.8	396.5	-18672.16376	60.1	0.032
10		2.365	-18675.93120	-18675.87776	-18675.81147	82.7	223.0	397.0	-18672.15730	77.1	0.035
11		2.312	-18675.92301	-18675.87540	-18675.81139	104.2	229.2	397.2	-18672.15001	96.3	0.038
12		2.258	-18675.91379	-18675.87352	-18675.81145	128.4	234.1	397.1	-18672.14192	117.5	0.041
13		2.204	-18675.90361	-18675.87210	-18675.81198	155.1	237.8	395.7	-18672.13306	140.8	0.043
14	**B'**	**2.150**	**-18675.88991**	**-18675.87667**	**-18675.83235**	**191.1**	**225.8**	**342.2**	**-18672.11610**	**185.3**	**0.034**
15		2.097	-18675.89144	-18675.87211	-18675.83292	187.0	237.8	340.7	-18672.11818	179.8	0.033
16		2.043	-18675.89472	-18675.86773	-18675.83142	178.4	249.3	344.6	-18672.12325	166.5	0.033
17		1.990	-18675.89891	-18675.86368	-18675.82884	167.4	259.9	351.4	-18672.12884	151.8	0.033
18		1.937	-18675.90376	-18675.86201	-18675.82501	154.7	264.3	361.5	-18672.13446	137.1	0.031
19		1.883	-18675.90908	-18675.86182	-18675.81979	140.7	264.8	375.2	-18672.14003	122.5	0.030
20		1.830	-18675.91476	-18675.86345	-18675.81316	125.8	260.5	392.6	-18672.14561	107.8	0.029
21		1.777	-18675.92069	-18675.86779	-18675.80526	110.3	249.2	413.3	-18672.15122	93.1	0.028
22		1.723	-18675.92676	-18675.87474	-18675.79686	94.3	230.9	435.4	-18672.15683	78.3	0.028
23		1.670	-18675.93285	-18675.88303	-18675.79159	78.3	209.1	449.2	-18672.16240	63.7	0.028
24		1.617	-18675.93881	-18675.89179	-18675.79334	62.7	186.1	444.6	-18672.16781	49.5	0.028
25		1.563	-18675.94441	-18675.90059	-18675.79884	48.0	163.0	430.2	-18672.17289	36.2	0.029
26		1.510	-18675.94936	-18675.90908	-18675.80533	35.0	140.7	413.1	-18672.17745	24.2	0.030
27		1.457	-18675.95332	-18675.91679	-18675.81173	24.6	120.5	396.3	-18672.18122	14.3	0.031
28		1.403	-18675.95580	-18675.92321	-18675.81746	18.1	103.6	381.3	-18672.18379	7.6	0.033
29	**C'**	**1.370**	**-18675.95635**	**-18675.92660**	**-18675.82081**	**16.6**	**94.7**	**372.5**	**-18672.18460**	**5.4**	**0.034**

Table S9. Potential energy characteristics of reaction-path of **dissociation of N_2 ligand** from the **$IrN_2O_2^-$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B"** to other minimum energy structure **C"** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

$IrN_2O_2^-$ – dissociation of N_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-N interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.780**	**-18675.96268**	**-18675.90247**	**-18675.81916**	**0.0**	**158.1**	**376.8**	**-18672.18667**	**0.0**	**0.020**
2		2.734	-18675.96137	-18675.89986	-18675.81512	3.5	164.9	387.4	-18672.18508	4.2	0.020
3		2.679	-18675.95909	-18675.89793	-18675.81265	9.4	170.0	393.9	-18672.18277	10.3	0.020
4		2.623	-18675.95564	-18675.89576	-18675.81017	18.5	175.7	400.4	-18672.17938	19.1	0.021
5		2.568	-18675.95095	-18675.89342	-18675.80761	30.8	181.9	407.2	-18672.17487	31.0	0.021
6		2.512	-18675.94496	-18675.89097	-18675.80501	46.5	188.3	414.0	-18672.16916	46.0	0.021
7		2.457	-18675.93760	-18675.88847	-18675.80240	65.9	194.9	420.8	-18672.16221	64.2	0.021
8		2.401	-18675.92876	-18675.88596	-18675.79989	89.1	201.4	427.4	-18672.15392	86.0	0.022
9		2.346	-18675.91836	-18675.88342	-18675.79748	116.4	208.1	433.8	-18672.14424	111.4	0.022
10	**B"**	**2.290**	**-18675.85354**	**-18675.88639**	**-18675.84968**	**286.6**	**200.3**	**296.7**	**-18672.08898**	**256.5**	**0.049**
11		2.238	-18675.86039	-18675.89301	-18675.85664	268.6	182.9	278.4	-18672.07712	287.6	0.053
12		2.185	-18675.86784	-18675.89098	-18675.85507	249.0	188.3	282.6	-18672.06899	309.0	0.054
13		2.133	-18675.87549	-18675.88831	-18675.85291	228.9	195.3	288.2	-18672.06032	331.7	0.055
14		2.090	-18675.88334	-18675.88493	-18675.85010	208.3	204.1	295.6	-18672.05165	354.5	0.056
15		2.040	-18675.89140	-18675.88078	-18675.84657	187.2	215.0	304.9	-18672.13297	141.0	0.020
16		1.990	-18675.89969	-18675.87581	-18675.84229	165.4	228.1	316.1	-18672.13959	123.6	0.022
17		1.940	-18675.90823	-18675.86998	-18675.83729	143.0	243.4	329.2	-18672.14666	105.1	0.024
18		1.890	-18675.91704	-18675.87487	-18675.83171	119.8	230.6	343.9	-18672.15415	85.4	0.026
19		1.840	-18675.92611	-18675.88088	-18675.82584	96.0	214.8	359.3	-18672.16203	64.7	0.029
20		1.790	-18675.93543	-18675.89092	-18675.82036	71.6	188.4	373.7	-18672.17025	43.1	0.031
21		1.740	-18675.94497	-18675.90109	-18675.81643	46.5	161.7	384.0	-18672.17874	20.8	0.034
22		1.690	-18675.95468	-18675.91131	-18675.81491	21.0	134.9	388.0	-18672.18740	-1.9	0.036
23		1.640	-18675.96449	-18675.92142	-18675.82379	-4.7	108.4	364.7	-18672.19611	-24.8	0.037
24		1.590	-18675.97429	-18675.93125	-18675.83246	-30.5	82.5	341.9	-18672.20472	-47.4	0.038
25		1.540	-18675.98397	-18675.94060	-18675.84118	-55.9	58.0	319.0	-18672.21311	-69.4	0.038
26		1.490	-18675.99335	-18675.94915	-18675.84969	-80.5	35.5	296.7	-18672.22114	-90.5	0.038
27		1.440	-18676.00221	-18675.95656	-18675.85764	-103.8	16.1	275.8	-18672.22870	-110.3	0.036
28		1.390	-18676.01022	-18675.96235	-18675.86453	-124.8	0.9	257.7	-18672.23562	-128.5	0.034
29		1.340	-18676.01691	-18675.96591	-18675.86982	-142.4	-8.5	243.8	-18672.24166	-144.4	0.032
30		1.290	-18676.02164	-18675.96889	-18675.87271	-154.8	-16.3	236.2	-18672.24630	-156.6	0.029
31	**C"**	**1.240**	**-18676.02343**	**-18675.97396**	**-18675.87203**	**-159.5**	**-29.6**	**238.0**	**-18672.24868**	**-162.8**	**0.026**

Table S10. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the PtO_4^{2-} molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtO_4^{2+} – dissociation of O_2

		DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	O-O interatomic distance ↓ [a.u.]	Energy E [kJ/mol]			Relative energy ΔE [a.u.]			Energy E [kJ/mol]	Relative energy ΔE -	T_1 [a.u.]
	Spin multiplicity →	1	3	5	1	3	1	3	5	1
1	**A 2.790**	**-19338.54845**	**-19338.50185**	**-19338.46686**	**0.0**	**122.3**	**214.2**	**-19334.69339**	**0.0**	**0.022**
2	2.740	-19338.54818	-19338.49137	-19338.46892	**0.7**	**149.9**	**208.8**	-19334.69236	**2.7**	0.022
3	2.690	-19338.54726	-19338.49066	-19338.46782	**3.1**	**151.7**	**211.7**	-19334.68742	**15.7**	0.047
4	2.640	-19338.54566	-19338.48967	-19338.46673	**7.3**	**154.3**	**214.6**	-19334.68482	**22.5**	0.044
5	2.590	-19338.54334	-19338.48834	-19338.46563	**13.4**	**157.8**	**217.4**	-19334.68201	**29.9**	0.040
6	2.540	-19338.54026	-19338.48667	-19338.46454	**21.5**	**162.2**	**220.3**	-19334.67885	**38.2**	0.036
7	2.490	-19338.53638	-19338.50285	-19338.46345	**31.7**	**119.7**	**223.2**	-19334.67519	**47.8**	0.034
8	2.440	-19338.53164	-19338.50301	-19338.46242	**44.1**	**119.3**	**225.9**	-19334.67082	**59.3**	0.032
9	2.390	-19338.52598	-19338.50308	-19338.46137	**59.0**	**119.1**	**228.6**	-19334.66561	**73.0**	0.031
10	2.340	-19338.51934	-19338.50299	-19338.46027	**76.4**	**119.4**	**231.5**	-19334.65950	**89.0**	0.031
11	2.290	-19338.51162	-19338.50269	-19338.45906	**96.7**	**120.2**	**234.7**	-19334.65248	**107.4**	0.031
12	2.240	-19338.50274	-19338.50212	-19338.45151	**120.0**	**121.6**	**254.5**	-19334.64401	**129.6**	0.031
13	2.190	-19338.49260	-19338.50123	-19338.45052	**146.6**	**124.0**	**257.1**	-19334.63555	**151.9**	0.032
14	2.140	-19338.48106	-19338.49993	-19338.44943	**176.9**	**127.4**	**260.0**	-19334.62551	**178.2**	0.033
15	2.090	-19338.46800	-19338.49813	-19338.44817	**211.2**	**132.1**	**263.3**	-19334.61435	**207.5**	0.034
16	2.040	-19338.45326	-19338.49576	-19338.44670	**249.9**	**138.3**	**267.2**	-19334.60196	**240.1**	0.035
17	B **1.990**	**-19338.41660**	**-19338.49275**	**-19338.44495**	**346.2**	**146.2**	**271.7**	**-19334.58697**	**279.4**	**0.028**
18	1.940	-19338.42742	-19338.48899	-19338.44287	**317.8**	**156.1**	**277.2**			
19	1.890	-19338.43919	-19338.48443	-19338.44047	**286.9**	**168.1**	**283.5**	-19334.56336	**341.4**	0.077
20	1.840	-19338.52828	-19338.50279	-19338.46325	**53.0**	**119.9**	**223.7**	-19334.66771	**67.4**	0.033
21	1.790	-19338.53612	-19338.49412	-19338.45831	**32.4**	**142.6**	**236.7**	-19334.67317	**53.1**	0.033
22	1.740	-19338.54399	-19338.51096	-19338.45251	**11.7**	**98.4**	**251.9**	-19334.67894	**37.9**	0.033
23	1.690	-19338.55184	-19338.52059	-19338.44826	**-8.9**	**73.1**	**263.0**	-19334.68490	**22.3**	0.033
24	1.640	-19338.55954	-19338.53138	-19338.45082	**-29.1**	**44.8**	**256.3**	-19334.69093	**6.5**	0.033
25	1.590	-19338.56700	-19338.54231	-19338.45757	**-48.7**	**16.1**	**238.6**	-19334.69691	**-9.2**	0.034
26	1.540	-19338.57413	-19338.55326	-19338.46606	**-67.4**	**-12.6**	**216.3**	-19334.70268	**-24.4**	0.035
27	1.490	-19338.58071	-19338.56401	-19338.48948	**-84.7**	**-40.9**	**154.8**	-19334.70808	**-38.6**	0.036
28	1.440	-19338.58651	-19338.57433	-19338.50774	**-99.9**	**-67.9**	**106.9**	-19334.71295	**-51.4**	0.037
29	1.390	-19338.59120	-19338.58371	-19338.51927	**-112.2**	**-92.6**	**76.6**	-19334.71696	**-61.9**	0.039
30	1.340	-19338.59437	-19338.59165	-19338.52999	**-120.6**	**-113.4**	**48.5**	-19334.71975	**-69.2**	0.040
31	C **1.290**	**-19338.59542**	**-19338.59745**	**-19338.53921**	**-123.3**	**-128.7**	**24.3**	**-19334.72069**	**-71.7**	**0.042**

Table S11. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **$PtNO_3^+$** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

$PtNO_3^+$ – dissociation of O_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓		O-O interatomic distance ↓ [Å]	Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.778**	**-19318.67346**	**-19318.62428**	**-19318.59980**	**0.0**	**129.1**	**193.4**	**-19314.83097**	**0.0**	**0.040**
2		2.745	-19318.67336	-19318.61855	-19318.59882	0.3	144.2	196.0	-19314.83961	-22.7	0.059
3		2.691	-19318.67252	-19318.61836	-19318.59711	2.5	144.7	200.5	-19314.83766	-17.6	0.058
4		2.636	-19318.67081	-19318.61779	-19318.59535	7.0	146.2	205.1	-19314.83514	-11.0	0.057
5		2.582	-19318.66818	-19318.61684	-19318.59365	13.9	148.7	209.5	-19314.83198	-2.7	0.056
6		2.527	-19318.66461	-19318.61546	-19318.59194	23.2	152.3	214.0	-19314.82804	7.7	0.056
7		2.473	-19318.66004	-19318.61371	-19318.59040	35.2	156.9	218.1	-19314.82327	20.2	0.056
8		2.418	-19318.65443	-19318.61159	-19318.58904	50.0	162.5	221.7	-19314.81755	35.2	0.056
9		2.364	-19318.64773	-19318.60917	-19318.58790	67.6	168.8	224.7	-19314.81070	53.2	0.056
10		2.309	-19318.63994	-19318.60659	-19318.58703	88.0	175.6	226.9	-19314.80251	74.7	0.055
11	**B**	**2.247**	**-19318.62052**	**-19318.62264**	**-19318.61312**	**139.0**	**133.4**	**158.4**	**-19314.79066**	**105.8**	**0.056**
12		2.150	-19318.63054	-19318.64031	-19318.62268	112.7	87.0	133.3	-19314.81067	53.3	0.060
13		2.100	-19318.63648	-19318.63814	-19318.62116	97.1	92.7	137.3	-19314.81999	28.8	0.061
14		2.050	-19318.64289	-19318.63500	-19318.61860	80.3	101.0	144.0	-19314.82849	6.5	0.061
15		2.000	-19318.64970	-19318.63085	-19318.61505	62.4	111.9	153.4	-19314.83602	-13.3	0.060
16		1.950	-19318.65686	-19318.62560	-19318.61046	43.6	125.7	165.4	-19314.84252	-30.3	0.058
17		1.900	-19318.66436	-19318.61918	-19318.60491	23.9	142.5	180.0	-19314.84790	-44.5	0.056
18		1.850	-19318.67217	-19318.65330	-19318.59873	3.4	52.9	196.2	-19314.85196	-55.1	0.052
19		1.800	-19318.68029	-19318.66249	-19318.59301	-17.9	28.8	211.2	-19314.85417	-60.9	0.046
20		1.750	-19318.68870	-19318.67211	-19318.59156	-40.0	3.5	215.0	-19314.87920	-126.6	0.063
21		1.700	-19318.69740	-19318.68194	-19318.59773	-62.9	-22.3	198.8	-19314.88649	-145.8	0.063
22		1.650	-19318.70633	-19318.69187	-19318.60733	-86.3	-48.3	173.6	-19314.89404	-165.6	0.063
23		1.600	-19318.71545	-19318.70183	-19318.60755	-110.2	-74.5	173.1	-19314.90138	-184.9	0.063
24		1.550	-19318.72465	-19318.71170	-19318.61961	-134.4	-100.4	141.4	-19314.90772	-201.5	0.062
25		1.500	-19318.73383	-19318.72131	-19318.63197	-158.5	-125.6	108.9	-19314.91225	-213.4	0.061
26		1.450	-19318.74284	-19318.73042	-19318.64444	-182.1	-149.5	76.2	-19314.91457	-219.5	0.058
27		1.400	-19318.75147	-19318.73875	-19318.65684	-204.8	-171.4	43.6	-19314.91507	-220.8	0.054
28		1.350	-19318.75940	-19318.74598	-19318.66895	-225.6	-190.4	11.8	-19314.91496	-220.5	0.049
29		1.300	-19318.76618	-19318.75171	-19318.68051	-243.4	-205.4	-18.5	-19314.91543	-221.8	0.044
30	**C**	**1.196**	**-19318.77308**	**-19318.76514**	**-19318.72076**	**-261.5**	**-240.7**	**-124.2**	**-19314.91708**	**-226.1**	**0.036**

Table S12. Potential energy characteristics of reaction-path of **dissociation of NO ligand** from the $PtNO_3^+$ molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B'** to other minimum energy structure **C'** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtN_2O_2 – dissociation of **NO**

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-O interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.840**	**-19318.67346**	**-19318.62428**	**-19318.59980**	**0.0**	**129.1**	**193.4**	**-19314.83097**	**0.0**	**0.040**
2		2.800	-19318.67330	-19318.62333	-19318.59832	0.4	131.6	197.3	-19314.84143	-27.5	0.062
3		2.750	-19318.67255	-19318.61763	-19318.59639	2.4	146.6	202.4	-19314.83886	-20.7	0.059
4		2.700	-19318.67119	-19318.62060	-19318.59434	6.0	138.8	207.7	-19314.83600	-13.2	0.057
5		2.650	-19318.66920	-19318.61871	-19318.59221	11.2	143.8	213.3	-19314.83286	-5.0	0.055
6		2.600	-19318.66655	-19318.61880	-19318.59004	18.2	143.5	219.0	-19314.82944	4.0	0.053
7		2.550	-19318.66320	-19318.61920	-19318.58788	26.9	142.5	224.7	-19314.82565	13.9	0.053
8		2.500	-19318.65911	-19318.61019	-19318.58579	37.7	166.1	230.2	-19314.82689	10.7	0.063
9		2.450	-19318.65424	-19318.62026	-19318.58386	50.5	139.7	235.2	-19314.82292	21.1	0.064
10		2.400	-19318.64853	-19318.62073	-19318.58220	65.4	138.4	239.6	-19314.81104	52.3	0.052
11		2.350	-19318.64192	-19318.62102	-19318.58088	82.8	137.7	243.1	-	-	-
12		2.300	-19318.63433	-19318.62110	-19318.57970	102.7	137.5	246.2	-	-	-
13	**B'**	**2.246**	**-19318.60046**	**-19318.63823**	**-19318.60248**	**191.7**	**92.5**	**186.4**	**-**	**-**	**-**
14		2.200	-19318.54575	-19318.64393	-19318.60900	335.3	77.5	169.2	-19314.98544	-405.6	0.095
15		2.155	-19318.60741	-19318.64201	-19318.60804	173.4	82.6	171.8	-19314.90866	-204.0	0.082
16		2.108	-19318.61402	-19318.63953	-19318.60663	156.1	89.1	175.5	-19314.86574	-91.3	0.072
17		2.061	-19318.62079	-19318.63642	-19318.60480	138.3	97.2	180.3	-19314.84215	-29.4	0.063
18		2.013	-19318.62768	-19318.63398	-19318.60246	120.2	103.7	186.4	-19314.80450	69.5	0.032
19		1.966	-19318.63470	-19318.63320	-19318.59950	101.8	105.7	194.2	-19314.82155	24.7	0.047
20		1.918	-19318.64184	-19318.63292	-19318.59579	83.0	106.4	203.9	-19314.81810	33.8	0.039
21		1.871	-19318.64903	-19318.63267	-19318.59116	64.1	107.1	216.1	-19314.81810	33.8	0.031
22		1.824	-19318.65621	-19318.63192	-19318.58554	45.3	109.1	230.8	-19314.82335	20.0	0.031
23		1.776	-19318.66335	-19318.63072	-19318.57880	26.5	112.2	248.5	-19314.82891	5.4	0.032
24		1.729	-19318.67044	-19318.63108	-19318.57522	7.9	111.3	257.9	-19314.83461	-9.6	0.032
25		1.682	-19318.67738	-19318.63410	-19318.57139	-10.3	103.4	268.0	-19314.84032	-24.6	0.033
26		1.634	-19318.68406	-19318.64001	-19318.57184	-27.8	87.8	266.8	-19314.84591	-39.2	0.034
27		1.587	-19318.69036	-19318.64807	-19318.57693	-44.4	66.7	253.5	-19314.85121	-53.1	0.034
28		1.539	-19318.69616	-19318.65702	-19318.58472	-59.6	43.2	233.0	-19314.85601	-65.7	0.035
29		1.492	-19318.70124	-19318.66607	-19318.59329	-72.9	19.4	210.5	-19314.86007	-76.4	0.037
30		1.445	-19318.70531	-19318.67471	-19318.60169	-83.6	-3.3	188.4	-19314.86309	-84.3	0.038
31		1.397	-19318.70802	-19318.68248	-19318.60934	-90.7	-23.7	168.3	-19314.86467	-88.5	0.040
32	**C'**	**1.351**	**-19318.70895**	**-19318.68871**	**-19318.61649**	**-93.2**	**-40.0**	**149.6**	**-19314.86431**	**-87.5**	**0.041**

Table S13. Potential energy characteristics of reaction-path of **dissociation of O_2 ligand** from the **PtN_2O_2** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B** to other minimum energy structure **C** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtN_2O_2 – dissociation of N_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓		O-O interatomic distance ↓ [Å]	Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.900**	**-19298.50132**	**-19298.47161**	**-19298.42858**	**0.0**	**78.0**	**191.0**	**-19294.68260**	**0.0**	**0.031**
2		2.890	-19298.50133	-19298.47254	-19298.42517	0.0	75.6	200.0	-19294.68250	0.3	0.031
3		2.840	-19298.50096	-19298.47268	-19298.41858	0.9	75.2	217.2	-19294.68171	2.3	0.031
4		2.790	-19298.50006	-19298.47090	-19298.41079	3.3	79.9	237.7	-19294.68043	5.7	0.031
5		2.740	-19298.49860	-19298.46764	-19298.40277	7.2	88.4	258.8	-19294.67865	10.4	0.030
6		2.690	-19298.49656	-19298.46330	-19298.39670	12.5	99.8	274.7	-19294.67634	16.4	0.030
7		2.640	-19298.49393	-19298.44070	-19298.39556	19.4	159.2	277.7	-19294.67350	23.9	0.030
8		2.590	-19298.49067	-19298.44571	-19298.39841	28.0	146.0	270.2	-19294.67008	32.9	0.030
9		2.540	-19298.48676	-19298.45062	-19298.40257	38.2	133.1	259.3	-19294.66607	43.4	0.030
10		2.490	-19298.48216	-19298.45424	-19298.40618	50.3	123.6	249.8	-19294.66143	55.6	0.030
11		2.440	-19298.47681	-19298.45660	-19298.40876	64.4	117.4	243.0	-19294.65612	69.5	0.030
12		2.390	-19298.47066	-19298.45786	-19298.41033	80.5	114.1	238.9	-19294.65010	85.3	0.030
13		2.340	-19298.42256	-19298.45841	-19298.41118	206.8	112.7	236.7	-19294.64700	93.5	0.068
14	**B**	**2.310**	**-19298.42282**	**-19298.46558**	**-19298.43190**	**206.1**	**93.9**	**182.3**	**-19294.64452**	**100.0**	**0.070**
15		2.290	-19298.42567	-19298.45873	-19298.41187	198.6	111.8	234.9	-19294.64767	91.7	0.058
16		2.240	-19298.42974	-19298.45914	-19298.41276	187.9	110.8	232.5	-19294.65496	72.6	0.057
17		2.190	-19298.43400	-19298.46006	-19298.41405	176.8	108.3	229.1	-19294.65864	62.9	0.053
18		2.140	-19298.44024	-19298.46228	-19298.41716	160.4	102.5	221.0	-19294.65525	71.8	0.047
19		2.090	-19298.44671	-19298.46483	-19298.41966	143.4	95.8	214.4	-19294.65562	70.8	0.044
20		2.040	-19298.45332	-19298.46587	-19298.42284	126.0	93.1	206.0	-19294.65748	66.0	0.041
21		1.990	-19298.46004	-19298.46687	-19298.42549	108.4	90.5	199.1	-19294.66045	58.2	0.038
22		1.940	-19298.46686	-19298.46729	-19298.42861	90.5	89.4	190.9	-19294.66426	48.2	0.036
23		1.890	-19298.47375	-19298.45143	-19298.41823	72.4	131.0	218.2	-19294.66871	36.5	0.034
24		1.840	-19298.48061	-19298.45494	-19298.41890	54.4	121.8	216.4	-19294.67361	23.6	0.033
25		1.790	-19298.48737	-19298.45798	-19298.41954	36.6	113.8	214.7	-19294.67883	9.9	0.032
26		1.740	-19298.49402	-19298.46062	-19298.42019	19.2	106.9	213.0	-19294.68421	-4.2	0.031
27		1.690	-19298.50046	-19298.46293	-19298.42087	2.3	100.8	211.2	-19294.68957	-18.3	0.031
28		1.640	-19298.50654	-19298.46496	-19298.42160	-13.7	95.5	209.3	-19294.69475	-31.9	0.030
29		1.590	-19298.51209	-19298.46675	-19298.42241	-28.3	90.8	207.2	-19294.69953	-44.4	0.029
30		1.540	-19298.51696	-19298.46830	-19298.42325	-41.0	86.7	205.0	-19294.70363	-55.2	0.028
31		1.490	-19298.52082	-19298.46961	-19298.42414	-51.2	83.3	202.6	-19294.70674	-63.4	0.028
32		1.440	-19298.52330	-19298.47068	-19298.42505	-57.7	80.5	200.3	-19294.70847	-67.9	0.026
33	**C**	**1.400**	**-19298.52340**	**-19298.47274**	**-19298.42415**	**-58.0**	**75.0**	**202.6**	**-19294.70851**	**-68.0**	**0.025**

Table S14. Potential energy characteristics of reaction-path of **dissociation of NO ligand** from the **PtN_2O_2** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B'** to other minimum energy structure **C'** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtN_2O_2 – dissociation of **NO**

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓		N-O interatomic distance ↓ [Å]	Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
		Spin multiplicity →	1	3	5	1	3	5	1	1	1
1	**A**	**2.836**	**-19298.50132**	**-19298.47161**	**-19298.42858**	**0.0**	**78.0**	**191.0**	**-19294.68260**	**0.0**	**0.031**
2		2.825	-19298.50133	-19298.47146	-19298.42832	0.0	78.4	191.7	-19294.68254	0.2	0.031
3		2.771	-19298.50087	-19298.47037	-19298.42700	1.2	81.3	195.1	-19294.71015	-72.3	0.078
4		2.716	-19298.49964	-19298.46871	-19298.42576	4.4	85.6	198.4	-19294.70738	-65.0	0.077
5		2.662	-19298.49762	-19298.46647	-19298.42466	9.7	91.5	201.3	-19294.70426	-56.9	0.076
6		2.607	-19298.49478	-19298.46364	-19298.42372	17.2	98.9	203.7	-19294.70070	-47.5	0.076
7		2.553	-19298.49109	-19298.46030	-19298.42297	26.9	107.7	205.7	-19294.69661	-36.8	0.075
8		2.498	-19298.48651	-19298.45674	-19298.42243	38.9	117.1	207.1	-19294.69187	-24.3	0.075
9		2.444	-19298.48102	-19298.45365	-19298.42209	53.3	125.2	208.0	-19294.68633	-9.8	0.075
10		2.389	-19298.47460	-19298.45152	-19298.42194	70.1	130.8	208.4	-19294.67974	7.5	0.075
11		2.335	-19298.46727	-19298.45039	-19298.42210	89.4	133.7	208.0	-19294.67169	28.7	0.074
12	**B'**	**2.280**	**-19298.45274**	**-19298.46281**	**-19298.44294**	**127.6**	**101.1**	**153.3**	**-19294.64091**	**109.5**	**0.057**
13		2.228	-19298.45708	-19298.46378	-19298.44828	116.2	98.6	139.3	-19294.64575	96.8	0.057
14		2.175	-19298.46205	-19298.46229	-19298.44769	103.1	102.5	140.8	-19294.65367	76.0	0.058
15		2.123	-19298.46763	-19298.46005	-19298.44619	88.5	108.4	144.8	-19294.66160	55.1	0.059
16		2.070	-19298.47367	-19298.45694	-19298.44373	72.6	116.5	151.2	-19294.66913	35.4	0.059
17		2.018	-19298.48008	-19298.46103	-19298.44032	55.8	105.8	160.2	-19294.67623	16.7	0.058
18		1.965	-19298.48681	-19298.46568	-19298.43588	38.1	93.6	171.8	-19294.68300	-1.0	0.057
19		1.913	-19298.49382	-19298.47139	-19298.43039	19.7	78.6	186.2	-19294.68963	-18.4	0.056
20		1.860	-19298.50110	-19298.47862	-19298.42421	0.6	59.6	202.5	-19294.69627	-35.9	0.055
21		1.808	-19298.50861	-19298.48741	-19298.41861	-19.1	36.5	217.2	-19294.70320	-54.1	0.055
22		1.755	-19298.51636	-19298.49691	-19298.41739	-39.5	11.6	220.4	-19294.71058	-73.5	0.054
23		1.703	-19298.52429	-19298.50680	-19298.42217	-60.3	-14.4	207.8	-19294.71851	-94.3	0.055
24		1.650	-19298.53236	-19298.51696	-19298.43201	-81.5	-41.0	182.0	-19294.72689	-116.3	0.055
25		1.598	-19298.54044	-19298.52724	-19298.44297	-102.7	-68.0	153.2	-19294.73561	-139.2	0.056
26		1.545	-19298.54840	-19298.53745	-19298.45443	-123.6	-94.9	123.1	-19294.74424	-161.8	0.057
27		1.493	-19298.55605	-19298.54735	-19298.46615	-143.7	-120.8	92.4	-19294.75204	-182.3	0.057
28		1.440	-19298.56312	-19298.55660	-19298.47776	-162.2	-145.1	61.9	-19294.75772	-197.2	0.055
29		1.388	-19298.56925	-19298.56477	-19298.48891	-178.4	-166.6	32.6	-19294.75995	-203.1	0.052
30		1.335	-19298.57394	-19298.57119	-19298.49906	-190.7	-183.4	6.0	-19294.76416	-214.1	0.056
31		1.283	-19298.57645	-19298.57512	-19298.50876	-197.3	-193.7	-19.5	-19294.77334	-238.2	0.068
32	**C'**	**1.262**	**-19298.57662**	**-19298.57575**	**-19298.51213**	**-197.7**	**-195.4**	**-28.4**	**-19294.77473**	**-241.9**	**0.070**

Table S15. Potential energy characteristics of reaction-path of **dissociation of N_2 ligand** from the **PtN_2O_2** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B"** to other minimum energy structure **C"** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done (because of high multireference nature we were unable to obtain result for some geometries). For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtN_2O_2 – dissociation of N_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-N interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.798**	**-19298.50132**	**-19298.47161**	**-19298.42858**	**0.0**	**78.0**	**191.0**	**-19294.68260**	**0.0**	**0.031**
2		2.774	-19298.50131	-19298.47129	-19298.42774	0.0	78.8	193.2	-19294.68238	0.6	0.031
3		2.718	-19298.50055	-19298.47035	-19298.42577	2.0	81.3	198.4	-19294.68125	3.5	0.031
4		2.661	-19298.49872	-19298.46913	-19298.42322	6.8	84.5	205.1	-19294.67920	8.9	0.032
5		2.605	-19298.49577	-19298.46773	-19298.42122	14.6	88.2	210.3	-19294.67617	16.9	0.032
6		2.549	-19298.49162	-19298.46615	-19298.41914	25.5	92.3	215.8	-19294.67213	27.5	0.032
7		2.493	-19298.48622	-19298.46450	-19298.41697	39.7	96.7	221.5	-19294.66702	40.9	0.032
8		2.436	-19298.47947	-19298.46280	-19298.41479	57.4	101.2	227.2	-19294.66077	57.3	0.032
9		2.380	-19298.47130	-19298.46108	-19298.41268	78.8	105.7	232.7	-19294.65334	76.8	0.033
10	**B"**	**2.350**	**-19298.43888**	**-19298.47220**	**-19298.45301**	**164.0**	**76.5**	**126.8**	**-19294.60143**	**213.1**	**0.053**
11		2.346	-19298.43691	-19298.48407	-19298.46151	169.1	45.3	104.5	-19294.67311	24.9	0.074
12		2.304	-19298.44291	-19298.48315	-19298.46072	153.4	47.7	106.6	-	-	-
13		2.263	-19298.44909	-19298.48190	-19298.45965	137.1	51.0	109.4	-	-	-
14		2.222	-19298.45546	-19298.48031	-19298.45825	120.4	55.2	113.1	-	-	-
15		2.180	-19298.46203	-19298.47833	-19298.45649	103.2	60.4	117.7	-19294.67030	32.3	0.045
16		2.139	-19298.46880	-19298.47592	-19298.45435	85.4	66.7	123.3	-19294.67471	20.7	0.045
17		2.098	-19298.47579	-19298.47305	-19298.45179	67.0	74.2	130.1	-19294.67942	8.4	0.045
18		2.057	-19298.48299	-19298.46969	-19298.44879	48.1	83.1	137.9	-19294.68440	-4.7	0.045
19		2.015	-19298.49042	-19298.46581	-19298.44537	28.6	93.2	146.9	-19294.68964	-18.5	0.045
20		1.974	-19298.49811	-19298.47322	-19298.44156	8.4	73.8	156.9	-19294.69511	-32.8	0.045
21		1.933	-19298.50608	-19298.47982	-19298.43753	-12.5	56.4	167.5	-19294.70083	-47.9	0.045
22		1.891	-19298.51434	-19298.48772	-19298.43335	-34.2	35.7	178.5	-19294.70675	-63.4	0.044
23		1.850	-19298.52289	-19298.49585	-19298.42950	-56.6	14.4	188.6	-19294.71296	-79.7	0.043
24		1.850	-19298.52299	-19298.49590	-19298.42944	-56.9	14.2	188.7	-19294.71302	-79.8	0.043
25		1.797	-19298.53442	-19298.50649	-19298.42549	-86.9	-13.6	199.1	-19294.72140	-101.8	0.042
26		1.743	-19298.54637	-19298.51723	-19298.42881	-118.3	-41.8	190.4	-19294.73035	-125.4	0.040
27		1.690	-19298.55884	-19298.52806	-19298.43748	-151.0	-70.2	167.6	-19294.74002	-150.8	0.038
28		1.637	-19298.57179	-19298.53877	-19298.44672	-185.0	-98.3	143.4	-19294.75058	-178.5	0.035
29		1.584	-19298.58519	-19298.54920	-19298.45702	-220.2	-125.7	116.3	-19294.76218	-208.9	0.033
30		1.531	-19298.59900	-19298.55914	-19298.47115	-256.4	-151.8	79.2	-19294.77490	-242.3	0.030
31		1.478	-19298.61307	-19298.56999	-19298.48622	-293.4	-180.3	39.6	-19294.78870	-278.6	0.028
32		1.425	-19298.62723	-19298.58654	-19298.50087	-330.6	-223.7	1.2	-19294.80339	-317.1	0.026
33		1.372	-19298.64112	-19298.60683	-19298.51641	-367.0	-277.0	-39.6	-19294.81854	-356.9	0.024
34		1.319	-19298.65421	-19298.62678	-19298.53591	-401.4	-329.4	-90.8	-19294.83342	-396.0	0.022
35		1.266	-19298.66563	-19298.64520	-19298.55783	-431.4	-377.7	-148.3	-19294.84696	-431.5	0.021
36		1.213	-19298.67408	-19298.66083	-19298.58086	-453.6	-418.8	-208.8	-19294.85764	-459.6	0.020
37	**C"**	**1.160**	**-19298.67756**	**-19298.67244**	**-19298.58290**	**-462.7**	**-449.3**	**-214.2**	**-19294.86346**	**-474.8**	**0.018**

Table S16. Potential energy characteristics of reaction-path of **dissociation of NO ligand** from the PtN_3O^- molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B'** to other minimum energy structure **C'** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done. For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtN_3O^- – dissociation of **NO**

No of step on the pathway ↓	N-O interatomic distance ↓ [Å]		DFT(M06-L)/ZORA Energy E [a.u.]			DFT(M06-L)/ZORA Relative energy ΔE [kJ/mol]			CCSD(T)/ZORA Energy E [a.u.]	CCSD(T)/ZORA Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.889**	**-19278.06078**	**-19278.02763**	**-19277.99943**	**0.0**	**87.0**	**161.1**	**-19274.28156**	**0.0**	**0.070**
2		2.850	-19278.06064	-19278.02686	-19277.99864	0.4	89.1	163.1	-19274.28028	3.4	0.069
3		2.800	-19278.05994	-19278.02549	-19277.99759	2.2	92.7	165.9	-19274.27839	8.3	0.068
4		2.750	-19278.05865	-19278.02367	-19277.99650	5.6	97.4	168.8	-19274.27615	14.2	0.067
5		2.700	-19278.05676	-19278.02132	-19277.99536	10.5	103.6	171.8	-19274.27345	21.3	0.066
6		2.650	-19278.05426	-19278.02044	-19277.99423	17.1	105.9	174.7	-19274.27029	29.6	0.065
7		2.600	-19278.05113	-19278.01832	-19277.99313	25.3	111.5	177.6	-19274.26665	39.2	0.065
8		2.550	-19278.04735	-19278.01605	-19277.99206	35.3	117.5	180.4	-19274.26246	50.2	0.064
9		2.500	-19278.04290	-19278.01364	-19277.99103	46.9	123.8	183.1	-19274.25766	62.8	0.064
10		2.450	-19278.03780	-19278.01114	-19277.99006	60.3	130.3	185.7	-19274.25208	77.4	0.063
11		2.400	-19278.03206	-19278.00865	-19277.98918	75.4	136.9	188.0	-19274.24544	94.8	0.062
12		2.350	-19278.02100	-19278.02166	-19277.99629	104.4	102.7	169.3	-19274.22335	152.8	0.037
13	**B'**	**2.352**	**-19278.02101**	**-19278.02158**	**-19277.99617**	**104.4**	**102.9**	**169.6**	**-19274.22342**	**152.6**	**0.037**
14		2.300	-19278.02314	-19278.02085	-19277.99657	98.8	104.8	168.6	-19274.22625	145.2	0.036
15		2.250	-19278.02633	-19278.01921	-19277.99617	90.4	109.1	169.6	-19274.23136	131.8	0.037
16		2.200	-19278.03015	-19278.01713	-19277.99544	80.4	114.6	171.5	-19274.23705	116.9	0.038
17		2.150	-19278.03445	-19278.01444	-19277.99417	69.1	121.7	174.9	-19274.24285	101.6	0.038
18		2.100	-19278.03912	-19278.02562	-19277.99224	56.9	92.3	180.0	-19274.24851	86.8	0.038
19		2.050	-19278.04409	-19278.02596	-19277.98961	43.8	91.4	186.9	-19274.25396	72.5	0.038
20		2.000	-19278.04930	-19278.02576	-19277.98627	30.1	92.0	195.6	-19274.25923	58.6	0.038
21		1.950	-19278.05472	-19278.02537	-19277.98220	15.9	93.0	206.3	-19274.26448	44.9	0.038
22		1.900	-19278.06031	-19278.02585	-19277.97769	1.2	91.7	218.2	-19274.26985	30.8	0.039
23		1.850	-19278.06605	-19278.02749	-19277.97369	-13.8	87.4	228.7	-19274.27543	16.1	0.040
24		1.800	-19278.07190	-19278.03520	-19277.97180	-29.2	67.2	233.6	-19274.28121	0.9	0.041
25		1.750	-19278.07786	-19278.04329	-19277.97322	-44.8	45.9	229.9	-19274.28714	-14.7	0.042
26		1.700	-19278.08387	-19278.05171	-19277.97815	-60.6	23.8	216.9	-19274.29317	-30.5	0.044
27		1.650	-19278.08986	-19278.06040	-19278.00180	-76.4	1.0	154.9	-19274.29921	-46.3	0.045
28		1.600	-19278.09573	-19278.06922	-19278.01150	-91.8	-22.2	129.4	-19274.30523	-62.2	0.047
29		1.550	-19278.10131	-19278.07802	-19278.02144	-106.4	-45.3	103.3	-19274.31115	-77.7	0.049
30		1.500	-19278.10640	-19278.08656	-19278.01467	-119.8	-67.7	121.1	-19274.31688	-92.7	0.051
31		1.450	-19278.11075	-19278.09454	-19278.04115	-131.2	-88.6	51.6	-19274.32234	-107.1	0.054
32		1.400	-19278.11401	-19278.10153	-19278.05033	-139.8	-107.0	27.4	-19274.32744	-120.5	0.057
33		1.350	-19278.11572	-19278.10696	-19278.05842	-144.2	-121.3	6.2	-19274.33191	-132.2	0.060
34	**C'**	**1.330**	**-19278.11583**	**-19278.10855**	**-19278.06125**	**-144.5**	**-125.4**	**-1.2**	**-19274.33344**	**-136.2**	**0.062**

Table S17. Potential energy characteristics of reaction-path of **dissociation of N_2 ligand** from the **PtN_3O^-** molecule. The reaction leads from **A** minimum structure (the highest formal oxidation state of a metal atom) through transition state **B"** to other minimum energy structure **C"** and so on (the rest of the path has not been studied in detail). The path was obtained by DFT(M06-L)/ZORA geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. For such calculated geometries (all singlets, M=1), single-point energies were calculated also for triplet (M=3) and quintet (M=5). For the same structures, CCSD(T)/ZORA single-point energy calculations were also done (because of high multireference nature we were unable to obtain result for some geometries). For all shown relative energies singlet-state energy of **A** isomer is set to zero. T_1 diagnostic values obtained for CCSD(T)/ZORA are additively shown (values greater than 0.045 are market by red).

PtN_3O^- – dissociation of N_2

			DFT(M06-L)/ZORA						CCSD(T)/ZORA		
No of step on the pathway ↓	N-N interatomic distance ↓ [Å]		Energy E [a.u.]			Relative energy ΔE [kJ/mol]			Energy E [a.u.]	Relative energy ΔE [kJ/mol]	T_1 -
	Spin multiplicity →		1	3	5	1	3	5	1	1	1
1	**A**	**2.867**	**-19278.06078**	**-19278.02763**	**-19277.99943**	**0.0**	**87.0**	**161.1**	**-19274.28156**	**0.0**	**0.070**
2		2.850	-19278.06079	-19278.02756	-19277.99902	0.0	87.2	162.2	-19274.28142	0.4	0.070
3		2.800	-19278.06032	-19278.02704	-19277.99775	1.2	88.6	165.5	-19274.28069	2.3	0.069
4		2.750	-19278.05912	-19278.02604	-19277.99641	4.4	91.2	169.0	-19274.27945	5.6	0.070
5		2.700	-19278.05715	-19278.02458	-19277.99506	9.5	95.1	172.5	-19274.27769	10.2	0.070
6		2.650	-19278.05438	-19278.02266	-19277.99374	16.8	100.1	176.0	-19274.27544	16.1	0.070
7		2.600	-19278.05078	-19278.02032	-19277.99248	26.3	106.2	179.3	-19274.27271	23.2	0.071
8		2.550	-19278.04630	-19278.01757	-19277.99130	38.0	113.5	182.4	-19274.26957	31.5	0.072
9		2.500	-19278.04091	-19278.01442	-19277.99022	52.2	121.7	185.3	-19274.26615	40.5	0.074
10		2.450	-19278.03455	-19278.01087	-19277.98923	68.9	131.1	187.9	-19274.26277	49.3	0.077
11		2.400	-19277.99992	-19278.04553	-19278.02919	159.8	40.1	82.9	-19274.26021	56.1	0.077
12	**B"**	**2.390**	**-19277.98995**	**-19278.04188**	**-19278.02216**	**186.0**	**49.6**	**101.4**	**-**	**-**	**-**
13		2.350	-19278.00632	-19278.04481	-19278.02865	143.0	41.9	84.4	-	-	-
14		2.300	-19278.01294	-19278.04371	-19278.02773	125.6	44.8	86.8	-	-	-
15		2.250	-19278.01976	-19278.04213	-19278.02640	107.7	49.0	90.3	-19274.27600	14.6	0.0709
16		2.200	-19278.02681	-19278.04008	-19278.02457	89.2	54.4	95.1	-19274.27370	20.6	0.066
17		2.150	-19278.03410	-19278.03750	-19278.02224	70.1	61.1	101.2	-19274.27584	15.0	0.063
18		2.100	-19278.04165	-19278.03437	-19278.01931	50.2	69.3	108.9	-19274.44517	-429.6	0.126
19		2.050	-19278.04946	-19278.03074	-19278.01578	29.7	78.9	118.1	-19274.28572	-10.9	0.060
20		2.000	-19278.05756	-19278.02685	-19278.01168	8.5	89.1	128.9	-19274.29188	-27.1	0.059
21		1.950	-19278.06601	-19278.05098	-19278.00719	-13.7	25.7	140.7	-19274.29830	-43.9	0.057
22		1.950	-19278.06601	-19278.05097	-19278.00720	-13.7	25.8	140.7	-19274.29830	-43.9	0.057
23		1.900	-19278.07483	-19278.06031	-19278.00267	-36.9	1.2	152.6	-19274.30454	-60.3	0.055
24		1.850	-19278.08405	-19278.07008	-19277.99879	-61.1	-24.4	162.8	-19274.31018	-75.1	0.052
25		1.800	-19278.09366	-19278.08018	-19277.99663	-86.3	-50.9	168.4	-19274.31460	-86.8	0.045
26		1.750	-19278.10368	-19278.09056	-19277.99681	-112.6	-78.2	168.0	-19274.31894	-98.1	0.040
27		1.700	-19278.11409	-19278.10114	-19277.99878	-140.0	-106.0	162.8	-19274.32911	-124.8	0.046
28		1.650	-19278.12485	-19278.11184	-19278.01995	-168.2	-134.0	107.2	-19274.33905	-150.9	0.048
29		1.600	-19278.13591	-19278.12250	-19278.03055	-197.3	-162.0	79.4	-19274.34824	-175.1	0.049
30		1.550	-19278.14720	-19278.13296	-19278.04135	-226.9	-189.5	51.0	-19274.35694	-197.9	0.047
31		1.500	-19278.15861	-19278.14299	-19278.05218	-256.9	-215.8	22.6	-19274.36557	-220.6	0.044
32		1.450	-19278.16997	-19278.15229	-19278.06279	-286.7	-240.2	-5.3	-19274.37451	-244.0	0.041
33		1.400	-19278.18099	-19278.16047	-19278.07280	-315.6	-261.7	-31.6	-19274.38394	-268.8	0.038
34		1.350	-19278.19129	-19278.16737	-19278.08171	-342.7	-279.8	-54.9	-19274.39363	-294.2	0.035
35		1.300	-19278.20029	-19278.17622	-19278.09515	-366.3	-303.1	-90.2	-19274.40286	-318.5	0.032
36		1.250	-19278.20708	-19278.18720	-19278.10378	-384.1	-331.9	-112.9	-19274.41045	-338.4	0.031
37		1.200	-19278.21044	-19278.19841	-19278.11234	-392.9	-361.3	-135.4	-19274.41477	-349.7	0.030
38		1.150	-19278.20849	-19278.20519	-19278.12182	-387.8	-379.1	-160.3	-19274.41373	-347.0	0.029
39	**C"**	**1.187**	**-19278.21054**	**-19278.20066**	**-19278.11519**	**-393.2**	**-367.3**	**-142.8**	**-19274.41513**	**-350.7**	**0.030**

Table S18. Testifying the validity of the Hammond's rule on investigated series of molecules: dependence between the **A→B_{TS}→C** reaction activation energy (E_{ACT})

and its energy (ΔE) for all investigated molecules: **A.** data obtained with DFT(M06-L)/ZORA approach **B.** at DFT(M06-L)/SO-ZORA level of theory. All data are divided to three families of reactions (O_2, NO, and N_2 dissociations).

A.

	Activation energy E_{ACT} [kJ/mol]			Reaction energy ΔE [kJ/mol]		
	O_2	NO	N_2	O_2	NO	N_2
OsO_4	406.3	-	-	269.9	-	-
$OsNO_3^-$	378.7	280.7	-	271.7	177.7	-
IrO_4^+	315.7	-	-	90.9	-	-
$IrNO_3$	308.5	207.8	-	100.7	-4.4	-
$IrN_2O_2^-$	277.1	191.1	286.6	121.0	16.6	-159.5
PtO_4^{2+}	346.2	-	-	-123.3	-	-
$PtNO_3^+$	191.7	*	-	-93.2	*	-
PtN_2O_2	127.6	127.6	164.0	-197.7	-197.7	-462.7
PtN_3O^-	-	104.4	186.0	-	-144.5	-393.2
$AuN_2O_2^+$	-	-	68.4	-	-	-822.7

* the obtained results are not unequivocal

B.

	Activation energy E_{ACT} [kJ/mol]			Reaction energy ΔE [kJ/mol]		
	O_2	NO	N_2	O_2	NO	N_2
OsO_4	344.6	-	-	264.0	-	-
$OsNO_3^-$	346.5	275.8	-	268.6	174.5	-
IrO_4^+	216.9	-	-	82.6	-	-
$IrNO_3$	227.1	200.7	-	95.4	-12.0	-
$IrN_2O_2^-$	209.5	185.9	171.5	117.8	13.2	-167.6
PtO_4^{2+}	56.4	-	-	-261.6	-	-
$PtNO_3^+$	93.0	79.2	-	-99.7	-520.3	-
PtN_2O_2	104.9	77.1	46.4	-63.0	-394.6	-706.2
PtN_3O^-	-	59.0	32.7	-	-308.7	-692.6

Table S19. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the **OsO_4** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

OsO_4 – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	O-O interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.776**	**-26.187456**	**0.0**
2	2.740	-26.187271	0.5
3	2.690	-26.186399	2.8
4	2.640	-26.184798	7.0
5	2.590	-26.182443	13.2
6	2.540	-26.179307	21.4
7	2.490	-26.175357	31.8
8	2.440	-26.170549	44.4
9	2.390	-26.164835	59.4
10	2.340	-26.158152	76.9
11	2.290	-26.150426	97.2
12	2.240	-26.141571	120.5
13	2.190	-26.131475	147.0
14	2.140	-26.120020	177.1
15	2.090	-26.107058	211.1
16	2.040	-26.092431	249.5
17	1.990	-26.075942	292.8
18	1.940	-26.078167	286.9
19	1.890	-26.072157	302.7
20	1.840	-26.065012	321.5
21	1.790	-26.056216	344.6
22	1.740	-26.059501	335.9
23	1.690	-26.066055	318.7
24	1.640	-26.072122	302.8
25	1.590	-26.077506	288.7
26	1.540	-26.081988	276.9
27	1.490	-26.085238	268.4
28	1.440	-26.086820	264.2
29	**C 1.428**	**-26.086891**	264.0

Table S20. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the $OsNO_3^-$ molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$OsNO_3^-$ – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	O-O interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.868**	**-26.307787**	**0.0**
2	2.840	-26.307693	0.2
3	2.790	-26.307048	1.9
4	2.740	-26.305784	5.3
5	2.690	-26.303884	10.2
6	2.640	-26.301339	16.9
7	2.590	-26.298129	25.4
8	2.540	-26.294221	35.6
9	2.490	-26.289583	47.8
10	2.440	-26.284175	62.0
11	2.390	-26.277944	78.4
12	2.340	-26.270824	97.0
13	2.290	-26.262748	118.3
14	2.240	-26.253625	142.2
15	2.190	-26.243365	169.1
16	2.140	-26.231827	199.4
17	2.090	-26.218886	233.4
18	2.040	-26.204380	271.5
19	1.990	-26.203118	274.8
20	1.940	-26.198248	287.6
21	1.890	-26.192211	303.4
22	1.840	-26.184802	322.9
23	1.790	-26.175815	346.5
24	1.740	-26.182534	328.9
25	1.690	-26.188422	313.4
26	1.640	-26.193817	299.2
27	1.590	-26.198506	286.9
28	1.540	-26.202274	277.0
29	1.490	-26.204741	270.5
30	1.440	-26.205467	268.6
31	**C 1.447**	**-26.205492**	**268.6**

Table S21. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of NO ligand** from the $OsNO_3^-$ molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$OsNO_3^-$ – dissociation of **NO**

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.785**	**-26.307787**	**0.0**
2		2.770	-26.307756	0.1
3		2.720	-26.307168	1.6
4		2.670	-26.305818	5.2
5		2.620	-26.303687	10.8
6		2.570	-26.300749	18.5
7		2.520	-26.296973	28.4
8		2.470	-26.292326	40.6
9		2.420	-26.286773	55.2
10		2.370	-26.280262	72.3
11		2.320	-26.272749	92.0
12		2.270	-26.264185	114.5
13		2.220	-26.254537	139.8
14		2.170	-26.243776	168.1
15		2.120	-26.231922	199.2
16		2.070	-26.219116	232.8
17		2.020	-26.206052	267.1
18	**B'**	**1.977**	**-26.202755**	**275.8**
19		1.970	-26.202775	275.7
20		1.920	-26.204074	272.3
21		1.870	-26.206699	265.4
22		1.820	-26.210228	256.1
23		1.770	-26.214392	245.2
24		1.720	-26.218969	233.2
25		1.670	-26.223738	220.7
26		1.620	-26.228462	208.3
27		1.570	-26.232892	196.6
28		1.520	-26.236727	186.6
29		1.470	-26.239625	179.0
30		1.420	-26.241170	174.9
31	**C'**	**1.402**	**-26.241307**	**174.5**

Table S22. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the **IrO_4^+** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

IrO_4^+ – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	O-O interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.759**	**-27.856155**	**0.0**
2	2.72	-27.855936	0.6
3	2.67	-27.855012	3.0
4	2.62	-27.853343	7.4
5	2.57	-27.850895	13.8
6	2.52	-27.847638	22.4
7	2.47	-27.843529	33.1
8	2.42	-27.838519	46.3
9	2.37	-27.832546	62.0
10	2.32	-27.825534	80.4
11	2.27	-27.817398	101.8
12	2.22	-27.808044	126.3
13	2.17	-27.797368	154.3
14	2.12	-27.796702	156.1
15	2.07	-27.793917	163.4
16	2.07	-27.794073	163.0
17	2.02	-27.790490	172.4
18	1.97	-27.785979	184.2
19	1.92	-27.780383	198.9
20	1.87	-27.773530	216.9
21	1.82	-27.783375	191.1
22	1.77	-27.785883	184.5
23	1.72	-27.793108	165.5
24	1.67	-27.800048	147.3
25	1.62	-27.806576	130.2
26	1.57	-27.812503	114.6
27	1.52	-27.817628	101.2
28	1.47	-27.821630	90.6
29	1.42	-27.824119	84.1
30	**C 1.385**	**-27.824683**	**82.6**

Table S23. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the **$IrNO_3$** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$IrNO_3$ – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	O-O interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.836**	**-28.256456**	**0.0**
2	2.820	-28.256421	0.1
3	2.770	-28.255905	1.4
4	2.720	-28.254750	4.5
5	2.670	-28.252942	9.2
6	2.620	-28.250451	15.8
7	2.570	-28.247269	24.1
8	2.520	-28.243352	34.4
9	2.470	-28.238661	46.7
10	2.420	-28.233150	61.2
11	2.370	-28.226758	78.0
12	2.320	-28.219412	97.3
13	2.270	-28.211044	119.2
14	2.220	-28.201555	144.1
15	2.170	-28.190837	172.3
16	2.120	-28.178770	204.0
17	2.070	-28.190595	172.9
18	2.020	-28.186999	182.4
19	1.970	-28.182468	194.3
20	1.920	-28.176865	209.0
21	1.870	-28.169949	227.1
22	1.820	-28.180152	200.3
23	1.770	-28.187113	182.1
24	1.720	-28.193846	164.4
25	1.670	-28.200237	147.6
26	1.620	-28.206140	132.1
27	1.570	-28.211376	118.4
28	1.520	-28.215707	107.0
29	1.470	-28.218774	98.9
30	1.420	-28.220116	95.4
31	**C 1.414**	**-28.220130**	**95.4**

Table S24. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of NO ligand** from the **$IrNO_3$** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$IrNO_3$ – dissociation of **NO**

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.755**	**-28.256456**	**0.0**
2		2.750	-28.256450	0.0
3		2.700	-28.255990	1.2
4		2.650	-28.254749	4.5
5		2.600	-28.252706	9.8
6		2.550	-28.249824	17.4
7		2.500	-28.246082	27.2
8		2.450	-28.241436	39.4
9		2.400	-28.235840	54.1
10		2.350	-28.229262	71.4
11		2.300	-28.221665	91.3
12		2.250	-28.213022	114.0
13		2.200	-28.203338	139.5
14		2.150	-28.192731	167.3
15	**B'**	**2.109**	**-28.180002**	**200.7**
16		2.050	-28.183561	191.4
17		2.000	-28.187135	182.0
18		1.950	-28.191813	169.7
19		1.900	-28.197287	155.3
20		1.850	-28.203209	139.8
21		1.800	-28.209443	123.4
22		1.750	-28.215944	106.4
23		1.700	-28.222613	88.9
24		1.650	-28.229337	71.2
25		1.600	-28.236006	53.7
26		1.550	-28.242426	36.8
27		1.500	-28.248395	21.2
28		1.450	-28.253634	7.4
29		1.400	-28.257797	-3.5
30		1.350	-28.260422	-10.4
31	**C'**	**1.315**	**-28.261028**	**-12.0**

Table S25. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the $IrN_2O_2^-$ molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$IrN_2O_2^-$ – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	O-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.904**	**-28.386052**	**0.0**
2		2.685	-28.380478	14.6
3		2.632	-28.377407	22.7
4		2.578	-28.373606	32.7
5		2.525	-28.369044	44.7
6		2.471	-28.363671	58.8
7		2.418	-28.357421	75.2
8		2.364	-28.350233	94.0
9		2.311	-28.342017	115.6
10		2.257	-28.332676	140.1
11		2.204	-28.325193	159.8
12		2.150	-28.323102	165.3
13		2.096	-28.320303	172.6
14		2.043	-28.316664	182.2
15		1.989	-28.312037	194.3
16		1.936	-28.306246	209.5
17		1.882	-28.306923	207.8
18		1.829	-28.308198	204.4
19		1.775	-28.314734	187.2
20		1.722	-28.321010	170.8
21		1.668	-28.326874	155.4
22		1.615	-28.332133	141.6
23		1.561	-28.336526	130.0
24		1.508	-28.339697	121.7
25		1.454	-28.341160	117.9
26	**C**	**1.445**	**-28.341192**	**117.8**

Table S26. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of NO ligand** from the $IrN_2O_2^-$ molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$IrN_2O_2^-$ – dissociation of **NO**

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.835**	**-28.386052**	**0.0**
2		2.796	-28.385826	0.6
3		2.742	-28.384845	3.2
4		2.689	-28.383083	7.8
5		2.635	-28.380508	14.6
6		2.582	-28.377099	23.5
7		2.528	-28.372823	34.7
8		2.475	-28.367637	48.3
9		2.421	-28.361513	64.4
10		2.367	-28.354410	83.1
11		2.314	-28.346312	104.3
12		2.260	-28.337223	128.2
13		2.207	-28.327245	154.4
14	**B'**	**2.154**	**-28.315229**	**185.9**
15		2.100	-28.317091	181.1
16		2.046	-28.320452	172.2
17		1.992	-28.324696	161.1
18		1.939	-28.329539	148.4
19		1.885	-28.334829	134.5
20		1.832	-28.340426	119.8
21		1.778	-28.346252	104.5
22		1.724	-28.352198	88.9
23		1.671	-28.358168	73.2
24		1.617	-28.364012	57.9
25		1.564	-28.369488	43.5
26		1.510	-28.374326	30.8
27		1.457	-28.378178	20.7
28		1.403	-28.380555	14.4
29	**C'**	**1.366**	**-28.381019**	**13.2**

Table S27. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of N_2 ligand** from the **$IrN_2O_2^-$** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$IrN_2O_2^-$ – dissociation of N_2

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-N interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.777**	**-28.386052**	**0.0**
2		2.74	-28.385824	0.6
3		2.69	-28.384767	3.4
4		2.64	-28.382826	8.5
5		2.59	-28.379947	16.0
6		2.54	-28.376103	26.1
7		2.49	-28.371248	38.9
8		2.44	-28.365326	54.4
9		2.39	-28.358280	72.9
10		2.34	-28.350044	94.5
11		2.29	-28.340531	119.5
12		2.24	-28.334705	134.8
13		2.19	-28.332315	141.1
14		2.14	-28.329208	149.2
15		2.09	-28.325365	159.3
16		2.04	-28.320717	171.5
17		1.99	-28.331369	143.6
18		1.94	-28.335336	133.2
19		1.89	-28.343825	110.9
20		1.84	-28.352572	87.9
21		1.79	-28.361601	64.2
22		1.74	-28.370871	39.9
23		1.69	-28.380353	15.0
24		1.64	-28.389965	-10.3
25		1.59	-28.399628	-35.6
26		1.54	-28.409222	-60.8
27		1.49	-28.418592	-85.4
28		1.44	-28.427502	-108.8
29		1.39	-28.435650	-130.2
30		1.34	-28.442569	-148.4
31		1.29	-28.447625	-161.7
32	**C"**	**1.236**	**-28.449870**	**-167.6**

Table S28. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the **PtO_4^+** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

PtO_4^{2+} – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	O-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.794**	**-29.385709**	**0.0**
2		2.750	-29.385514	0.5
3		2.700	-29.384590	2.9
4		2.675	-29.384393	3.5
5		2.650	-29.384784	2.4
6		2.625	-29.385130	1.5
7		2.600	-29.385435	0.7
8		2.575	-29.385692	0.0
9		2.550	-29.385902	-0.5
10		2.525	-29.386056	-0.9
11		2.500	-29.386135	-1.1
12	**MIN**	**2.472**	**-29.386197**	**-1.3**
13		2.450	-29.386156	-1.2
14		2.400	-29.385999	-0.8
15		2.350	-29.385488	0.6
16		2.300	-29.384503	3.2
17		2.250	-29.383271	6.4
18		2.200	-29.381591	10.8
19		2.150	-29.379408	16.5
20		2.100	-29.376720	23.6
21		2.050	-29.373366	32.4
22		2.000	-29.369303	43.1
23		1.950	-29.364214	56.4
24		1.900	-29.372781	33.9
25		1.850	-29.375275	27.4
26		1.800	-29.398596	-33.8
27		1.750	-29.399056	-35.0
28		1.700	-29.400893	-39.9
29		1.650	-29.404741	-50.0
30		1.600	-29.411027	-66.5
31		1.550	-29.419631	-89.1
32		1.500	-29.429890	-116.0
33		1.450	-29.441049	-145.3
34		1.400	-29.452406	-175.1
35		1.350	-29.463325	-203.8
36		1.300	-29.473033	-229.3
37		1.260	-29.479274	-245.7
38		1.240	-29.481711	-252.1
39		1.220	-29.483549	-256.9
40		1.200	-29.484820	-260.2
41		1.180	-29.485354	-261.6

*minimum C is missing

Table S29. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of N_2 ligand** from the **$PtNO_3^+$** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$PtNO_3^+$ – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	O-O interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.846**	**-30.081189**	**0.0**
2	2.800	-30.080946	0.6
3	2.750	-30.080129	2.8
4	2.700	-30.078703	6.5
5	2.650	-30.076651	11.9
6	2.600	-30.073949	19.0
7	2.550	-30.070558	27.9
8	2.500	-30.066439	38.7
9	2.500	-30.066884	37.6
10	2.45	-30.067165	36.8
11	2.400	-30.067154	36.8
12	2.350	-30.066822	37.7
13	2.300	-30.066134	39.5
14	2.300	-30.066131	39.5
15	2.250	-30.065020	42.5
16	2.200	-30.063446	46.6
17	2.150	-30.061326	52.1
18	2.100	-30.058586	59.3
19	2.050	-30.055142	68.4
20	2.000	-30.050800	79.8
21	1.970	-30.050015	81.8
22	1.920	-30.048424	86.0
23	1.870	-30.046651	90.7
24	1.870	-30.046586	90.8
25	1.860	-30.046178	91.9
26	1.850	-30.045770	93.0
27	1.830	-30.066226	39.3
28	1.820	-30.067727	35.3
29	1.780	-30.074256	18.2
30	1.730	-30.081234	-0.1
31	1.680	-30.088073	-18.1
32	1.630	-30.094661	-35.4
33	1.590	-30.100875	-51.7
34	1.540	-30.106594	-66.7
35	1.490	-30.111601	-79.8
36	1.440	-30.115620	-90.4
37	1.400	-30.118284	-97.4
38	**C 1.355**	**-30.119164**	**-99.7**

Table S30. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of NO ligand** from the $PtNO_3^+$ molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

$PtNO_3^+$ – dissociation of **NO**

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.780**	**-30.081189**	**0.0**
2		2.750	-30.081062	0.3
3		2.700	-30.080305	2.3
4		2.650	-30.078827	6.2
5		2.600	-30.076603	12.0
6		2.550	-30.069394	31.0
7		2.500	-30.068736	32.7
8		2.450	-30.067854	35.0
9		2.400	-30.066738	37.9
10		2.350	-30.065354	41.6
11		2.300	-30.063663	46.0
12		2.250	-30.061625	51.4
13		2.200	-30.059164	57.8
14		2.150	-30.056238	65.5
15		2.100	-30.052714	74.8
16		2.120	-30.054187	70.9
17		2.110	-30.053460	72.8
18		2.100	-30.052513	75.3
19		2.080	-30.051011	79.2
20		2.070	-30.073724	19.6
21		2.060	-30.074081	18.7
22		2.050	-30.074503	17.6
23		2.000	-30.076808	11.5
24		1.950	-30.080116	2.8
25		1.900	-30.084530	-8.8
26		1.850	-30.089843	-22.7
27		1.750	-30.094524	-35.0
28		1.700	-30.102771	-56.7
29		1.650	-30.110990	-78.2
30		1.600	-30.120152	-102.3
31		1.600	-30.120149	-102.3
32		1.550	-30.129443	-126.7
33		1.500	-30.138601	-150.7
34		1.450	-30.147464	-174.0
35		1.500	-30.138601	-150.7
36		1.450	-30.147464	-174.0
37		1.400	-30.155942	-196.3
38		1.300	-30.192256	-291.6
39		1.250	-30.241009	-419.6
40		1.200	-30.259255	-467.5
41		1.150	-30.272901	-503.3
42		1.100	-30.279236	-520.0
43	**C'**	**1.093**	**-30.279345**	**-520.3**

Table S31. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of O_2 ligand** from the **PtN_2O_2** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

PtN_2O_2 – dissociation of O_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	O-O interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.905**	**-30.481406**	**0.0**
2	2.850	-30.481086	0.8
3	2.800	-30.480223	3.1
4	2.750	-30.478837	6.7
5	2.700	-30.476889	11.9
6	2.650	-30.474348	18.5
7	2.600	-30.471198	26.8
8	2.550	-30.467409	36.7
9	2.500	-30.461497	52.3
10	2.450	-30.461575	52.1
11	2.400	-30.461390	52.6
12	2.350	-30.460902	53.8
13	2.300	-30.460065	56.0
14	2.250	-30.458814	59.3
15	2.200	-30.457099	63.8
16	2.150	-30.454843	69.7
17	2.100	-30.451965	77.3
18	2.050	-30.448489	86.4
19	2.000	-30.446493	91.7
20	1.950	-30.444873	95.9
21	1.900	-30.443039	100.7
22	1.890	-30.442621	101.8
23	1.880	-30.442189	103.0
24	1.870	-30.441711	104.2
25	1.850	-30.461786	51.5
26	1.840	-30.463134	48.0
27	1.870	-30.441711	104.2
28	1.870	-30.441462	104.9
29	1.860	-30.461120	53.3
30	1.850	-30.461798	51.5
31	1.850	-30.461795	51.5
32	1.800	-30.468502	33.9
33	1.750	-30.475088	16.6
34	1.700	-30.481455	-0.1
35	1.650	-30.487497	-16.0
36	1.600	-30.493037	-30.5
37	1.550	-30.497938	-43.4
38	1.500	-30.501888	-53.8
39	1.450	-30.504525	-60.7
40	**C 1.405**	**-30.505406**	**-63.0**

Table S32. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of NO ligand** from the PtN_2O_2 molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

PtN_2O_2 – dissociation of **NO**

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.839**	**-30.481406**	**0.0**
2		2.800	-30.481220	0.5
3		2.750	-30.480035	3.6
4		2.700	-30.479167	5.9
5		2.650	-30.477134	11.2
6		2.600	-30.474488	18.2
7		2.550	-30.471470	26.1
8		2.500	-30.468735	33.3
9		2.450	-30.465214	42.5
10		2.400	-30.464217	45.1
11		2.350	-30.462931	48.5
12		2.300	-30.461319	52.7
13		2.250	-30.459338	57.9
14		2.200	-30.456937	64.2
15		2.200	-30.456934	64.3
16		2.150	-30.454077	71.8
17		2.100	-30.452030	77.1
18		2.050	-30.455245	68.7
19		2.000	-30.459580	57.3
20		1.950	-30.465457	41.9
21		1.950	-30.464868	43.4
22		1.900	-30.472016	24.7
23		1.850	-30.479940	3.8
24		1.800	-30.488214	-17.9
25		1.750	-30.496744	-40.3
26		1.700	-30.505545	-63.4
27		1.650	-30.514595	-87.1
28		1.600	-30.523767	-111.2
29		1.550	-30.533035	-135.6
30		1.500	-30.538430	-149.7
31		1.450	-30.556064	-196.0
32		1.400	-30.573137	-240.8
33		1.350	-30.589685	-284.3
34		1.300	-30.604981	-324.4
35		1.250	-30.618027	-358.7
36		1.200	-30.627505	-383.6
37		1.150	-30.631658	-394.5
38	**C'**	**1.145**	**-30.631696**	**-394.6**

Table S33. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of N_2 ligand** from the **PtN_2O_2** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

PtN_2O_2 – dissociation of N_2

No of step on the pathway	DFT(M06-L)/SO-ZORA		
	N-N interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.797**	**-30.481406**	**0.0**
2	2.770	-30.481292	0.3
3	2.720	-30.480468	2.5
4	2.670	-30.478814	6.8
5	2.620	-30.476291	13.4
6	2.570	-30.474449	18.3
7	2.520	-30.474827	17.3
8	**MIN 2.479**	**-30.474936**	**17.0**
9	2.470	-30.474926	17.0
10	2.420	-30.474704	17.6
11	2.370	-30.474124	19.1
12	2.320	-30.473113	21.8
13	2.270	-30.471645	25.6
14	2.220	-30.469629	30.9
15	2.170	-30.467015	37.8
16	2.120	-30.463734	46.4
17	2.095	-30.474878	17.1
18	2.070	-30.476548	12.8
19	2.045	-30.478530	7.6
20	2.020	-30.480822	1.5
21	1.970	-30.485456	-10.6
22	1.920	-30.493632	-32.1
23	1.870	-30.503338	-57.6
24	1.820	-30.513411	-84.0
25	1.770	-30.523986	-111.8
26	1.720	-30.534632	-139.7
27	1.670	-30.546555	-171.0
28	1.620	-30.558982	-203.7
29	1.570	-30.571880	-237.5
30	1.520	-30.585213	-272.5
31	1.470	-30.598882	-308.4
32	1.420	-30.612707	-344.7
33	1.370	-30.635231	-403.9
34	1.320	-30.665060	-482.2
35	1.270	-30.693077	-555.7
36	1.220	-30.717807	-620.7
37	1.170	-30.737278	-671.8
38	**C" 1.095**	**-30.750391**	**-706.2**

Table S34. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of NO ligand** from the PtN_3O^- molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

PtN_3O^- – dissociation of **NO**

No of step on the pathway	DFT(M06-L)/SO-ZORA			
	N-O interatomic distance [Å]		Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A**	**2.893**	**-30.613934**	**0.0**
2		2.850	-30.613735	0.5
3		2.800	-30.612983	2.5
4		2.750	-30.611660	6.0
5		2.700	-30.609746	11.0
6		2.650	-30.607223	17.6
7		2.600	-30.604087	25.9
8		2.550	-30.600715	34.7
9		2.500	-30.595257	49.0
10		2.450	-30.594748	50.4
11		2.400	-30.593338	54.1
12		2.350	-30.594121	52.0
13		2.300	-30.593568	53.5
14		2.250	-30.593110	54.7
15		2.200	-30.592639	55.9
16		2.150	-30.592307	56.8
17		2.100	-30.591462	59.0
18		2.050	-30.600094	36.3
19		2.000	-30.604650	24.4
20		2.000	-30.604650	24.4
21		1.950	-30.610003	10.3
22		1.900	-30.615510	-4.1
23		1.900	-30.615512	-4.1
24		1.850	-30.621170	-19.0
25		1.800	-30.626952	-34.2
26		1.750	-30.632815	-49.6
27		1.700	-30.638736	-65.1
28		1.650	-30.644650	-80.6
29		1.600	-30.650666	-96.4
30		1.550	-30.656749	-112.4
31		1.500	-30.663026	-128.9
32		1.450	-30.674750	-159.7
33		1.400	-30.700617	-227.6
34		1.350	-30.712198	-258.0
35		1.300	-30.721988	-283.7
36		1.250	-30.728887	-301.8
37	**C'**	**1.201**	**-30.731528**	**-308.7**

Table S35. Potential energy characteristics (total bonding energies and relative energies) of reaction-path of **dissociation of N_2 ligand** from the **PtN_3O^-** molecule. The path was obtained by geometry optimization calculations with an arbitrary constraint on chosen interatomic distance (indicated in the table) and allowing all others to optimize. Calculations were performed with DFT(M06-L)/SO-ZORA approach (included spin-orbit approximation) with unrestricted spin and noncollinear spin polarization approximation. All energies in kJ/mol are relative - the energy of **A** isomer is set to zero.

PtN_3O^- – dissociation of N_2

PtN_3O^-	DFT(M06-L)/SO-ZORA		
No of step on the pathway	N-N interatomic distance [Å]	Energy E [a.u.]	Relative Energy ΔE [kJ/mol]
1	**A 2.868**	**-30.613934**	**0.0**
2	2.850	-30.613889	0.1
3	2.800	-30.613295	1.7
4	2.750	-30.611974	5.1
5	2.700	-30.609896	10.6
6	2.650	-30.607029	18.1
7	2.600	-30.603343	27.8
8	2.550	-30.608910	13.2
9	2.500	-30.609131	12.6
10	2.450	-30.609046	12.8
11	2.400	-30.608616	14.0
12	2.350	-30.607804	16.1
13	2.300	-30.605538	22.0
14	2.250	-30.603856	26.5
15	2.200	-30.601466	32.7
16	2.100	-30.605558	22.0
17	2.050	-30.611910	5.3
18	2.000	-30.617411	-9.1
19	2.000	-30.617447	-9.2
20	1.950	-30.625890	-31.4
21	1.900	-30.634690	-54.5
22	1.900	-30.634623	-54.3
23	1.850	-30.643910	-78.7
24	1.800	-30.652712	-101.8
25	1.750	-30.663052	-129.0
26	1.700	-30.673201	-155.6
27	1.650	-30.683157	-181.7
28	1.600	-30.695363	-213.8
29	1.550	-30.705081	-239.3
30	1.500	-30.713952	-262.6
31	1.450	-30.726756	-296.2
32	1.400	-30.736881	-322.8
33	1.350	-30.747731	-351.3
34	1.300	-30.757128	-376.0
35	1.250	-30.764595	-395.6
36	1.200	-30.768797	-406.6
37	1.150	-30.870277	-673.0
38	1.100	-30.877626	-692.3
39	**C" 1.095**	**-30.877714**	**-692.6**

Table S36. Harmonic frequencies computed for isomers of investigated compounds contains metal atoms at higher available oxidation state. Equilibrium geometries and frequencies were computed at DFT(M06-L)/SO-ZORA level of theory.

OsO_4 minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
342.1	56.97	4.89
342.3	57.07	4.90
342.5	56.95	4.89
346.7	0.11	0.01
346.8	0.05	0.00
1001.5	535.16	134.34
1001.6	534.95	134.30
1001.6	534.99	134.31
1020.2	0.01	0.00

$OsNO_3^-$ minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
315.2	71.50	5.65
315.4	71.28	5.63
336.2	58.22	4.91
382.3	38.02	3.64
382.3	37.84	3.63
901.0	972.51	219.63
901.1	972.61	219.68
920.5	465.30	107.36
1075.2	324.69	87.51

IrO_4^+ minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
339.7	9.39	0.80
339.7	9.76	0.83
339.9	9.81	0.84
340.4	0.47	0.04
340.5	0.10	0.01
994.8	0.01	0.00
1007.3	146.34	36.95
1007.4	146.31	36.94
1007.4	146.25	36.93

$IrNO_3$ minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
312.3	30.69	2.40
312.5	30.67	2.40
339.0	24.80	2.11
380.7	9.25	0.88
380.7	9.25	0.88
935.6	161.81	37.95
939.3	439.74	103.53
939.4	439.71	103.54
1065.8	80.42	21.48

$IrN_2O_2^-$ minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
300.5	44.97	3.39
339.1	50.58	4.30
340.8	0.03	0.00
354.5	114.77	10.20
412.5	7.96	0.82
845.5	840.98	178.22
848.1	583.62	124.07
979.6	596.20	146.39
1021.3	146.76	37.57

PtO_4^{2+} minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
312.1	0.16	0.01
312.3	0.01	0.00
314.6	5.82	0.46
316.8	4.59	0.36
318.2	3.59	0.29
892.0	0.05	0.01
927.6	0.09	0.02
929.4	0.19	0.04
948.2	2.36	0.56

$PtNO_3^+$ minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
292.8	5.21	0.38
292.9	5.26	0.39
323.2	1.45	0.12
353.1	0.64	0.06
353.2	0.65	0.06
882.2	29.28	6.48
908.9	95.15	21.68
909.0	95.27	21.71
972.5	2.06	0.50

PtN_2O_2 minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
286.6	18.96	1.36
319.3	0.00	0.00
324.3	17.18	1.40
334.3	31.30	2.62
391.0	0.13	0.01
836.2	207.22	43.43
850.1	341.61	72.79
938.1	110.52	25.99
966.3	34.11	8.26

PtN_3O^- minimum A

Frequency [cm^{-1}]	Dipole strength [10^{-40}·esu²·cm²]	Absorption intensity [km/mole]
307.1	24.17	1.86
307.1	23.97	1.85
348.5	108.08	9.44
369.8	15.34	1.42
370.0	15.21	1.41
753.2	609.89	115.15
885.1	465.68	103.32
885.3	464.38	103.05
921.0	58.19	13.43

Table S37. Lengths of selected metal-ligand bonds (r) and their bond-order analysis according to Mayer, Gopinathan-Jug (G-J) and Nalewajski-Mrozek. N-M(1) - bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP2], 3-index set; N-M (2) - bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP2], 4-index set; N-M(3) - bond-orders calculated from valence indices based on partitioning of tr(PΔP]. In the last column the ratio of N-M(1) indices for M≡N and M=O bonds is presented. Result are presented for **A** isomers (containing metal atoms at the highest oxidation states) of chosen molecules.

A. Structures optimized with DFT(M06-L)/ZORA/TZ2P in ADF.

Molecule	Bond	r [Å]	MAYER	G-J	N-M (1)	N-M (2)	N-M (3)	ratio
$OsNO_3^-$ (**A**)	Os=O	1.748	1.424	1.245	1.519	2.398	1.542	1.49
	Os≡N	1.685	2.362	2.007	2.261	2.786	2.156	
	∑Os(all)	**-**	**6.633**	**5.742**	**6.817**	**9.980**	**6.782**	
OsO_4 (**A**)	Os=O	1.706	1.589	1.433	1.676	2.169	1.577	
	∑Os(all)	**-**	**6.355**	**5.731**	**6.702**	**8.677**	**6.310**	
$IrNO_3$ (**A**)	Ir=O	1.727	1.436	1.194	1.392	2.006	1.313	1.45
	Ir≡N	1.676	2.149	1.843	2.020	2.102	1.789	
	∑Ir(all)	**-**	**6.456**	**5.424**	**6.196**	**8.121**	**5.727**	
PtN_2O_2 (**A**)	Pt=O	1.775	1.236	0.930	0.988	1.706	0.916	1.43
	Pt≡N	1.718	1.791	1.436	1.415	1.619	1.208	
	∑Pt(all)	**-**	**6.053**	**4.733**	**4.807**	**6.650**	**4.248**	
AuN_3O (**A**)	Au=O	1.839	1.015	0.688	0.698	1.522	0.619	1.37
	Au≡N	1.789	1.442	1.038	0.955	1.305	0.760	
	∑Au(all)	**-**	**5.340**	**3.801**	**3.563**	**5.437**	**2.900**	
HgN_4 (**A**)	Hg≡N	1.905	1.121	0.693	0.664	1.155	0.468	
	∑Hg(all)	**-**	**4.485**	**2.772**	**2.656**	**4.618**	**1.872**	
HgN_3O^+ (**A**)	Hg=O	1.910	0.877	0.532	0.554	1.017	0.404	1.30
	Hg≡N	1.896	1.134	0.740	0.719	0.584	0.465	
	∑Hg(all)	**-**	**4.280**	**2.752**	**2.711**	**2.770**	**1.799**	

B. Results from single-point calculations DFT(M06-L)/ZORA level of theory with TZ2P basis set in ADF for equilibrium geometries optimized at DFT(M06-L)/ZORA with SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca.

Molecule	Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	ratio
$OsNO_3^-$ (**A**)	Os=O	1.744	1.423	1.246	1.520	2.400	1.542	1.49
	Os≡N	1.684	2.362	2.004	2.259	2.791	2.156	
	∑Os(all)	**-**	**6.631**	**5.741**	**6.818**	**9.992**	**6.783**	
OsO_4 (**A**)	Os=O	1.698	1.585	1.432	1.677	2.175	1.578	
	∑Os(all)	**-**	**6.340**	**5.729**	**6.708**	**8.698**	**6.314**	
$IrNO_3$ (**A**)	Ir=O	1.722	1.436	1.195	1.394	2.010	1.314	1.45
	Ir≡N	1.674	2.151	1.841	2.019	2.109	1.788	
	∑Ir(all)	**-**	**6.458**	**5.425**	**6.200**	**8.139**	**5.730**	
PtN_2O_2 (**A**)	Pt=O	1.763	1.237	0.935	0.994	1.710	0.919	1.42
	Pt≡N	1.715	1.798	1.435	1.415	1.635	1.209	
	∑Pt(all)	**-**	**6.070**	**4.740**	**4.818**	**6.689**	**4.256**	
AuN_3O (**A**)	Au=O	1.831	1.018	0.690	0.701	1.536	0.622	1.37
	Au≡N	1.782	1.449	1.042	0.960	1.317	0.764	
	∑Au(all)	**-**	**5.365**	**3.815**	**3.580**	**5.486**	**2.914**	
HgN_4 (**A**)	Hg≡N	1.889	1.137	0.702	0.674	1.181	0.475	
	∑Hg(all)	**-**	**4.546**	**2.808**	**2.695**	**4.723**	**1.902**	

It is clear that the formal cumulative BOs for diverse species fall down in the series Os^{VIII} > Ir^{IX} > Pt^{X} etc., thus correlating with the anomalous increase of the metal-ligand distances (see main manuscript).

Table S38. Lengths of selected metal-ligand bonds (r) and their bond-order analysis according to Mayer, Gopinathan-Jug (G-J) and Nalewajski-Mrozek. N-M(1) -

bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP2], 3-index set; N-M (2) - bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP2], 4-index set; N-M(3) - bond-orders calculated from valence indices based on partitioning of tr(PΔP]. In the last column the ratio of N-M(1) indices for M≡N and M=O bonds is presented. Result are presented for **A**, **C**, **C'** and **C"** isomers (of molecules containing platinum atoms presented in this work). Data for geometries optimized with DFT(M06-L)/ZORA and SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca.

A. Results from single-point calculations DFT(M06-L)/ZORA level of theory with TZ2P basis set in ADF for equilibrium geometries optimized at DFT(M06-L)/ZORA with SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca. Results for PtN_3O^-.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	N-M(1) ratio
PtN_3O^- (**A**)	M=1	Pt=O	1.813	1.194	0.887	0.946	1.696	0.889	
		Pt≡N	1.746	1.645	1.264	1.278	1.586	1.081	1.35
		∑Pt(all)	**-**	**6.126**	**4.680**	**4.780**	**6.452**	**4.131**	
	M=3	Pt=O	1.813	1.158	0.857	0.947	1.666	0.872	
		Pt≡N (2x)	1.746	1.530	1.179	1.094	1.391	0.910	1.15
		Pt≡N	1.746	1.619	1.250	1.278	1.566	1.089	1.35
		∑Pt(all)	**-**	**5.836**	**4.465**	**4.414**	**6.014**	**3.781**	
	M=5	Pt=O	1.813	1.154	0.843	0.925	1.594	0.846	
		Pt≡N (2x)	1.746	1.416	1.108	1.028	1.297	0.862	1.11
		Pt≡N	1.746	1.477	1.155	1.099	1.375	0.915	1.19
		∑Pt(all)	**-**	**5.462**	**4.215**	**4.080**	**5.563**	**3.485**	
PtN_3O^- (**C'**)	M=1	Pt=O	2.055	0.520	0.357	0.393	0.648	0.338	
		Pt≡N	1.739	1.905	1.508	1.560	1.832	1.408	3.96
		∑Pt(all)	**-**	**5.172**	**4.018**	**4.215**	**5.103**	**3.732**	
	M=3	Pt=O	1.929	0.841	0.644	0.703	0.790	0.579	
		Pt≡N (2x)	2.055	0.543	0.369	0.398	0.667	0.347	0.57
		Pt≡N	1.739	1.751	1.403	1.386	1.630	1.197	1.97
		∑Pt(all)	**-**	**4.876**	**3.809**	**3.821**	**4.670**	**3.287**	
	M=5	Pt=O	1.929	0.831	0.633	0.650	0.743	0.547	
		Pt≡N (2x)	2.055	0.440	0.288	0.318	0.606	0.274	0.49
		Pt≡N	1.739	1.523	1.262	1.235	1.403	1.074	1.90
		∑Pt(all)	**-**	**4.310**	**3.452**	**3.457**	**4.166**	**2.980**	
PtN_3O^- (**C"**)	M=1	Pt=O	1.825	1.303	1.022	1.203	1.656	1.137	
		Pt≡N	1.730	1.903	1.621	1.784	1.919	1.530	1.48
		∑Pt(all)	**-**	**4.451**	**3.518**	**3.938**	**4.602**	**3.457**	
	M=3	Pt=O	2.076	0.622	0.437	0.476	0.514	0.395	
		Pt≡N (2x)	1.825	1.179	0.973	1.159	1.516	1.087	2.44
		Pt≡N	1.730	1.811	1.549	1.532	1.665	1.337	3.22
		∑Pt(all)	**-**	**4.143**	**3.334**	**3.576**	**4.126**	**3.158**	
	M=5	Pt=O	2.076	0.577	0.406	0.443	0.472	0.367	
		Pt≡N (2x)	1.825	1.091	0.978	1.187	1.366	1.079	2.68
		Pt≡N	1.730	1.510	1.258	1.217	1.395	1.095	2.75
		∑Pt(all)	**-**	**3.669**	**2.998**	**3.236**	**3.626**	**2.865**	

B. Results from single-point calculations DFT(M06-L)/ZORA level of theory with TZ2P basis set in ADF for equilibrium geometries optimized at DFT(M06-L)/ZORA with SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca. Results for PtN_2O_2.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	N-M(1) ratio
PtN_2O_2 (**A**)	M=1	Pt=O	1.763	1.237	0.935	0.994	1.710	0.919	
		Pt≡N	1.715	1.798	1.435	1.415	1.635	1.209	1.42
		∑Pt(all)	**-**	**6.070**	**4.740**	**4.818**	**6.689**	**4.256**	
	M=3	Pt=O	1.763	1.261	0.968	1.052	1.764	0.979	
		Pt≡N	1.715	1.610	1.296	1.207	1.379	1.022	1.15
		∑Pt(all)	**-**	**5.743**	**4.527**	**4.518**	**6.285**	**4.002**	
	M=5	Pt=O	1.763	1.149	0.898	0.965	1.540	0.888	
		Pt≡N	1.715	1.528	1.233	1.137	1.383	0.977	1.18
		∑Pt(all)	**-**	**5.354**	**4.262**	**4.204**	**5.847**	**3.730**	
PtN_2O_2 (**C**)	M=1	Pt=O	1.970	0.642	0.476	0.541	0.871	0.485	
		Pt≡N	1.701	1.978	1.588	1.631	1.844	1.456	3.02
		∑Pt(all)	**-**	**5.239**	**4.126**	**4.343**	**5.430**	**3.883**	
	M=3	Pt=O	1.970	0.652	0.490	0.594	0.924	0.538	
		Pt≡N	1.701	1.729	1.426	1.364	1.520	1.213	2.30
		∑Pt(all)	**-**	**4.761**	**3.833**	**3.914**	**4.888**	**3.502**	
	M=5	Pt=O	1.970	0.420	0.302	0.337	0.549	0.296	
		Pt≡N	1.701	1.741	1.453	1.429	1.594	1.297	4.24
		∑Pt(all)	**-**	**4.322**	**3.510**	**3.531**	**4.286**	**3.186**	
PtN_2O_2 (**C'**)	M=1	Pt=O (1)	1.764	1.320	1.026	1.140	1.677	1.100	1.49
		Pt=O (2)	2.051	0.618	0.459	0.495	0.692	0.430	1.72
		Pt≡N (1)	1.698	1.950	1.634	1.700	1.880	1.525	
		Pt≡N (2)	1.927	1.013	0.809	0.854	0.850	0.723	
		∑Pt(all)	**-**	**4.901**	**3.928**	**4.188**	**5.099**	**3.777**	
	M=3	Pt=O (1)	1.764	1.372	1.075	1.175	1.673	1.131	1.41
		Pt=O (2)	2.051	0.528	0.375	0.403	0.628	0.350	1.69
		Pt≡N (1)	1.698	1.972	1.684	1.654	1.757	1.466	
		Pt≡N (2)	1.927	0.844	0.661	0.679	0.736	0.574	
		∑Pt(all)	**-**	**4.715**	**3.795**	**3.912**	**4.794**	**3.521**	
	M=5	Pt=O (1)	1.764	1.200	1.034	1.242	1.521	1.201	1.22
		Pt=O (2)	2.051	0.374	0.256	0.274	0.537	0.240	2.31
		Pt≡N (1)	1.698	1.820	1.559	1.519	1.649	1.379	
		Pt≡N (2)	1.927	0.802	0.620	0.633	0.682	0.533	
		∑Pt(all)	**-**	**4.197**	**3.469**	**3.668**	**4.389**	**3.354**	
PtN_2O_2 (**C"**)	M=1	Pt=O	1.750	1.464	1.246	1.493	1.847	1.429	
		Pt≡N	2.087	0.650	0.470	0.525	0.520	0.439	0.35
		∑Pt(all)	**-**	**4.229**	**3.433**	**4.034**	**4.734**	**3.734**	
	M=3	Pt=O	1.750	1.476	1.270	1.386	1.691	1.318	
		Pt≡N	2.087	0.585	0.412	0.457	0.481	0.384	0.33
		∑Pt(all)	**-**	**4.122**	**3.364**	**3.688**	**4.345**	**3.404**	
	M=5	Pt=O	1.750	1.319	1.172	1.346	1.577	1.330	
		Pt≡N	2.087	0.484	0.351	0.388	0.366	0.327	0.29
		∑Pt(all)	**-**	**3.606**	**3.045**	**3.469**	**3.886**	**3.313**	

C. Results from single-point calculations DFT(M06-L)/ZORA level of theory with TZ2P basis set in ADF for equilibrium geometries optimized at DFT(M06-L)/ZORA with SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca. Results for $PtNO_3^+$.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	N-M(1) ratio
$PtNO_3^+$ (**A**)	M=1	Pt=O	1.728	1.228	0.977	1.096	1.741	0.966	
		Pt≡N	1.698	1.799	1.484	1.540	1.639	1.241	1.41
		∑Pt(all)	**-**	**5.522**	**4.437**	**4.836**	**6.848**	**4.148**	
	M=3	Pt=O	1.728	1.279	1.026	1.120	1.759	1.004	
		Pt≡N	1.728	1.225	0.987	1.071	1.663	0.937	0.96
		∑Pt(all)	**-**	**5.384**	**4.371**	**4.563**	**6.511**	**3.915**	
	M=5	Pt=O	1.698	1.668	1.380	1.310	1.447	1.050	
		Pt≡N	1.728	1.217	0.993	1.077	1.621	0.940	0.82
		∑Pt(all)	**-**	**4.964**	**4.069**	**4.253**	**6.012**	**3.643**	
$PtNO_3^+$ (**C**)	M=1	Pt=O	1.717	1.304	1.033	1.215	1.738	1.103	1.51
		Pt=O (2x)	1.944	0.638	0.495	0.588	0.866	0.502	3.12
		Pt≡N	1.670	2.027	1.717	1.838	1.883	1.534	
		∑Pt(all)	**-**	**4.607**	**3.740**	**4.230**	**5.353**	**3.640**	
	M=3	Pt=O	1.717	1.408	1.134	1.248	1.701	1.159	1.43
		Pt=O (2x)	1.944	0.517	0.393	0.453	0.715	0.376	3.93
		Pt≡N	1.670	2.023	1.733	1.780	1.827	1.508	
		∑Pt(all)	**-**	**4.464**	**3.653**	**3.934**	**4.959**	**3.418**	
	M=5	Pt=O	1.717	1.301	1.085	1.250	1.596	1.123	1.22
		Pt=O (2x)	1.944	0.444	0.345	0.388	0.552	0.324	3.91
		Pt≡N	1.670	1.729	1.490	1.519	1.636	1.277	
		∑Pt(all)	**-**	**3.917**	**3.265**	**3.546**	**4.336**	**3.048**	
$PtNO_3^+$ (**C'**)	M=1	Pt=O (2x)	1.721	1.313	1.088	1.318	1.744	1.200	0.70
		Pt=O	2.095	0.497	0.383	0.438	0.583	0.356	2.11
		Pt≡N	1.957	1.013	0.835	0.921	0.739	0.729	
		∑Pt(all)	**-**	**4.137**	**3.394**	**3.994**	**4.809**	**3.485**	
	M=3	Pt=O (2x)	1.721	1.392	1.174	1.333	1.705	1.225	0.59
		Pt=O	2.095	0.459	0.347	0.386	0.549	0.316	2.03
		Pt≡N	1.957	0.884	0.716	0.783	0.679	0.618	
		∑Pt(all)	**-**	**4.126**	**3.411**	**3.834**	**4.638**	**3.384**	
	M=5	Pt=O (2x)	1.721	1.331	1.151	1.296	1.579	1.168	0.51
		Pt=O	2.095	0.402	0.297	0.325	0.505	0.267	2.03
		Pt≡N	1.957	0.759	0.611	0.660	0.636	0.523	
		∑Pt(all)	**-**	**3.824**	**3.209**	**3.577**	**4.300**	**3.128**	

D. Results from single-point calculations DFT(M06-L)/ZORA level of theory with TZ2P basis set in ADF for equilibrium geometries optimized at DFT(M06-L)/ZORA with SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca. Results for PtO_4^{2+}.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)
PtO_4^{2+} (**A**)	M=1	Pt=O	1.708	1.432	1.214	1.209	0.728	0.932
		∑Pt(all)	**-**	**5.727**	**4.857**	**4.837**	**2.911**	**3.727**
	M=3	Pt=O	1.708	1.338	1.150	1.151	0.664	0.878
		∑Pt(all)	**-**	**5.353**	**4.601**	**4.604**	**2.656**	**3.514**
	M=5	Pt=O (2x)	1.708	1.233	1.079	1.088	0.558	0.816
		Pt=O (2x)	1.708	1.228	1.073	1.139	0.684	0.879
		∑Pt(all)	**-**	**4.922**	**4.305**	**4.453**	**2.483**	**3.390**
PtO_4^{2+} (**C**)	M=1	Pt=O (2x)	1.689	1.574	1.392	1.441	0.965	1.134
		Pt=O (2x)	1.957	0.779	0.665	0.711	0.184	0.540
		∑Pt(all)	**.**	**4.704**	**4.113**	**4.304**	**2.298**	**3.347**
	M=3	Pt=O (2x)	1.689	1.616	1.450	1.502	0.990	1.174
		Pt=O (2x)	1.957	0.588	0.497	0.536	0.048	0.401
		∑Pt(all)	**-**	**4.408**	**3.895**	**4.077**	**2.074**	**3.151**
	M=5	Pt=O (2x)	1.689	1.517	1.417	1.588	0.948	1.230
		Pt=O (2x)	1.957	0.412	0.338	0.366	0.020	0.273
		∑Pt(all)	**-**	**3.858**	**3.510**	**3.909**	**1.935**	**3.006**

It is clear that the formal cumulative BOs is the largest for the quasi-tetrahedral minimum **A** of interest (computed as a singlet state), thus corresponding to the largest formal OS of the metal. Other minima (**C**, **C'**) or higher multiplicities of **A** show much smaller BO values.

Table S39. Lengths of selected metal-ligand bonds (r) and their bond-order analysis according to Mayer, Gopinathan-Jug (G-J) and Nalewajski-Mrozek. N-M(1) - bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP2], 3-index set; N-M (2) - bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP2], 4-index set; N-M(3) - bond-orders calculated from valence indices based on partitioning of tr(PΔP]. In the last column the ratio of N-M(1) indices for M≡N and M=O bonds is presented. Result are presented for **A**, **C**, **C'** and **C"** isomers (of molecules containing platinum atoms presented in this work). Data for geometries optimized with DFT(M06-L)/SO-ZORA and TZ2P basis set in ADF.

A. Results from single-point calculations DFT(M06-L)/ZORA/TZ2P in ADF for equilibrium geometries optimized with DFT(M06-L)/SO-ZORA/TZ2P in ADF. Results for PtN_3O^-.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	N-M(1) ratio
PtN_3O^- (**A**)	M=1	Pt=O	1.815	1.093	0.808	0.906	1.977	0.912	
		Pt≡N	1.747	1.726	1.299	1.305	2.039	1.200	1.44
		∑Pt(all)	**-**	**6.271**	**4.706**	**4.821**	**8.095**	**4.510**	
	M=3	Pt=O	1.815	1.120	0.848	0.981	2.012	0.991	
		Pt≡N (2x)	1.747	1.603	1.215	1.181	1.872	1.089	1.20
		Pt≡N	1.747	1.624	1.234	1.151	1.880	1.065	1.17
		∑Pt(all)	**-**	**5.951**	**4.511**	**4.495**	**7.637**	**4.234**	
	M=5	Pt=O	1.815	1.087	0.822	0.937	1.896	0.945	
		Pt≡N (2x)	1.747	1.524	1.172	1.117	1.791	1.049	1.19
		Pt≡N	1.747	1.425	1.099	1.021	1.662	0.953	1.09
		∑Pt(all)	**-**	**5.561**	**4.265**	**4.192**	**7.140**	**3.997**	
PtN_3O^- (**C'**)	M=1	Pt=O	2.861	0.209	0.256	0.285	0.527	0.264	
		Pt≡N (1)	1.727	2.021	1.481	1.582	2.070	1.587	
		Pt≡N (2)	1.739	1.933	1.422	1.522	2.020	1.526	
		Pt≡N (3)	2.020	0.987	0.689	0.736	0.846	0.661	
		∑Pt(all)	**-**	**5.150**	**3.847**	**4.125**	**5.463**	**4.037**	
	M=3	Pt=O	-	-	-	-	-	-	
		Pt≡N (1)	1.727	2.028	1.518	1.805	2.231	1.804	
		Pt≡N (2)	1.739	1.887	1.442	1.403	1.814	1.402	
		Pt≡N (3)	2.020	0.789	0.534	0.529	0.718	0.476	
		∑Pt(all)	**-**	**4.830**	**3.625**	**3.877**	**5.157**	**3.811**	
	M=5	Pt=O	-	-	-	-	-	-	
		Pt≡N (1)	1.727	1.802	1.400	1.497	1.842	1.536	
		Pt≡N (2)	1.739	1.722	1.358	1.383	1.711	1.411	
		Pt≡N (3)	2.020	0.734	0.500	0.504	0.688	0.458	
		∑Pt(all)	**-**	**4.370**	**3.359**	**3.494**	**4.583**	**3.506**	
PtN_3O^- (**C"**)	M=1	Pt=O	1.778	1.410	1.044	1.336	1.538	1.471	
		Pt≡N	1.704	2.077	1.764	1.748	1.865	1.821	1.31
		∑Pt(all)	**-**	**3.719**	**2.936**	**3.615**	**3.927**	**3.816**	
	M=3	Pt=O	1.778	1.418	1.101	1.332	1.524	1.495	
		Pt≡N	1.704	2.077	1.764	1.748	1.865	1.821	1.31
		∑Pt(all)	**-**	**3.490**	**2.872**	**3.088**	**3.396**	**3.323**	
	M=5	Pt=O	1.778	1.083	0.925	1.236	1.276	1.423	
		Pt≡N	1.704	1.712	1.469	1.429	1.446	1.585	1.16
		∑Pt(all)	**-**	**2.801**	**2.413**	**2.687**	**2.748**	**3.028**	

B. Results from single-point calculations DFT(M06-L)/ZORA/TZ2P in ADF for equilibrium geometries optimized with DFT(M06-L)/SO-ZORA/TZ2P in ADF. Results for PtN_2O_2.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	N-M(1) ratio
PtN_2O_2 (**A**)	M=1	Pt=O	1.766	1.237	0.935	0.993	1.707	0.919	1.43
		Pt≡N	1.716	1.794	1.435	1.415	1.634	1.209	
		∑Pt(all)	**-**	**6.061**	**4.740**	**4.817**	**6.682**	**4.255**	
	M=3	Pt=O	1.766	1.262	0.967	1.052	1.762	0.980	1.15
		Pt≡N	1.716	1.605	1.296	1.206	1.377	1.021	
		∑Pt(all)	**-**	**5.734**	**4.526**	**4.516**	**6.277**	**4.001**	
	M=5	Pt=O	1.766	1.149	0.896	0.964	1.537	0.887	1.18
		Pt≡N	1.716	1.525	1.234	1.138	1.383	0.978	
		∑Pt(all)	**-**	**5.347**	**4.260**	**4.204**	**5.839**	**3.731**	
PtN_2O_2 (**C**)	M=1	Pt=O (2x)	1.971	0.641	0.476	0.541	0.873	0.485	3.01
		Pt≡N (2x)	1.704	1.970	1.587	1.630	1.842	1.456	
		∑Pt(all)	**-**	**5.221**	**4.126**	**4.342**	**5.430**	**3.882**	
	M=3	Pt=O (2x)	1.971	0.651	0.491	0.594	0.927	0.539	2.29
		Pt≡N (2x)	1.704	1.723	1.425	1.362	1.517	1.212	
		∑Pt(all)	**-**	**4.748**	**3.832**	**3.913**	**4.887**	**3.501**	
	M=5	Pt=O (2x)	1.971	0.419	0.302	0.337	0.550	0.296	4.23
		Pt≡N (2x)	1.704	1.735	1.452	1.427	1.591	1.296	
		∑Pt(all)	**-**	**4.309**	**3.508**	**3.530**	**4.284**	**3.185**	
PtN_2O_2 (**C'**)	M=1	Pt=O (1)	1.756	1.408	1.033	1.161	1.622	1.166	1.64
		Pt=O (2)	2.933	0.232	0.282	0.309	0.289	0.267	2.15
		Pt≡N (1)	1.685	2.172	1.787	1.900	2.069	1.777	
		Pt≡N (2)	2.155	0.820	0.615	0.665	0.513	0.567	
		∑Pt(all)	**-**	**4.632**	**3.717**	**4.034**	**4.493**	**3.778**	
	M=3	Pt=O (1)	1.756	1.420	1.091	1.161	1.573	1.141	
		Pt=O (2)	-	-	-	-	-	-	
		Pt≡N (1)	1.684	2.183	1.819	1.886	2.002	1.723	1.62
		Pt≡N (2)	2.153	0.699	0.499	0.498	0.478	0.421	
		∑Pt(all)	**-**	**4.477**	**3.584**	**3.725**	**4.268**	**3.438**	
	M=5	Pt=O (1)	1.756	1.192	0.959	1.097	1.380	1.090	
		Pt=O (2)	-	-	-	-	-	-	
		Pt≡N (1)	1.685	1.938	1.693	1.583	1.667	1.454	1.44
		Pt≡N (2)	2.155	0.656	0.468	0.479	0.482	0.411	
		∑Pt(all)	**-**	**3.952**	**3.283**	**3.333**	**3.752**	**3.106**	
PtN_2O_2 (**C"**)	M=1	Pt=O	1.703	1.734	1.478	1.817	1.965	1.736	
		Pt≡N	-	-	-	-	-	-	
		∑Pt(all)	**-**	**3.465**	**2.962**	**3.643**	**3.935**	**3.480**	
	M=3	Pt=O	1.703	1.565	1.307	1.501	1.740	1.393	
		Pt≡N	-	-	-	-	-	-	
		∑Pt(all)	**-**	**3.129**	**2.622**	**3.010**	**3.484**	**2.793**	
	M=5	Pt=O	1.703	1.258	1.103	1.292	1.457	1.207	
		Pt≡N	-	-	-	-	-	-	
		∑Pt(all)	**-**	**2.513**	**2.213**	**2.593**	**2.919**	**2.422**	

C. Results from single-point calculations DFT(M06-L)/ZORA/TZ2P in ADF for equilibrium geometries optimized with DFT(M06-L)/SO-ZORA/TZ2P in ADF. Results for $PtNO_3^+$.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)	N-M(1) ratio
$PtNO_3^+$ (**A**)	M=1	Pt=O	1.731	1.348	1.075	1.100	1.308	0.931	1.39
		Pt≡N	1.699	1.822	1.562	1.525	1.052	1.201	
		∑Pt(all)	**-**	**5.868**	**4.786**	**4.826**	**4.976**	**3.994**	
	M=3	Pt=O (2x)	1.731	1.217	0.988	0.990	1.119	0.826	1.37
		Pt=O	1.731	1.378	1.111	1.242	1.430	1.069	1.09
		Pt≡N	1.699	1.703	1.452	1.359	0.991	1.063	
		∑Pt(all)	**-**	**5.514**	**4.539**	**4.580**	**4.659**	**3.784**	
	M=5	Pt=O	1.731	1.264	1.040	1.079	1.179	0.904	
		Pt≡N	1.699	1.353	1.164	1.091	0.814	0.852	1.01
		∑Pt(all)	**-**	**2.240**	**2.245**	**2.514**	**2.363**	**2.496**	
$PtNO_3^+$ (**C**)	M=1	Pt=O	1.722	1.467	1.171	1.234	1.421	1.077	
		Pt=O (2x)	1.948	0.716	0.577	0.635	0.619	0.527	
		Pt≡N	1.673	2.020	1.803	1.831	1.412	1.492	1.48
		∑Pt(all)	**-**	**4.918**	**4.129**	**4.335**	**4.071**	**3.622**	
	M=3	Pt=O	1.722	1.426	1.190	1.239	1.369	1.087	
		Pt=O (2x)	1.948	0.498	0.382	0.403	0.371	0.327	
		Pt≡N	1.673	2.111	1.889	2.117	1.709	1.764	1.71
		∑Pt(all)	**-**	**4.533**	**3.842**	**4.161**	**3.819**	**3.505**	
	M=5	Pt=O	1.722	1.232	1.036	1.174	1.200	1.023	
		Pt=O (2x)	1.948	0.500	0.396	0.430	0.424	0.351	
		Pt≡N	1.673	1.856	1.717	1.695	1.306	1.365	1.44
		∑Pt(all)	**-**	**4.089**	**3.545**	**3.729**	**3.354**	**3.091**	
$PtNO_3^+$ (**C'**)	M=1	Pt=O (1)	1.756	1.633	1.383	1.528	1.596	1.368	
		Pt=O (2)	2.933	0.243	0.279	0.308	0.063	0.249	
		Pt≡N (1)	1.685	1.691	1.432	1.571	1.623	1.402	1.03
		Pt≡N (2)	2.155	0.716	0.562	0.621	0.243	0.501	
		∑Pt(all)	**-**	**4.282**	**3.656**	**4.029**	**3.525**	**3.520**	
	M=3	Pt=O (1)	1.756	1.536	1.306	1.341	1.437	1.186	
		Pt=O (2)	-	-	-	-	-	-	
		Pt≡N (1)	1.685	1.603	1.341	1.441	1.574	1.288	1.07
		Pt≡N (2)	2.155	0.723	0.582	0.606	0.166	0.471	
		∑Pt(all)	**-**	**4.087**	**3.468**	**3.639**	**3.127**	**3.141**	
	M=5	Pt=O (1)	1.756	1.257	1.105	1.243	1.309	1.134	
		Pt=O (2)	-	-	-	-	-	-	
		Pt≡N (1)	1.685	1.427	1.272	1.382	1.435	1.253	1.11
		Pt≡N (2)	2.1545	0.6978	0.5787	0.6148	0.2079	0.4826	
		∑Pt(all)	**-**	**3.590**	**3.178**	**3.477**	**2.931**	**3.056**	

D. Results from single-point calculations DFT(M06-L)/ZORA/TZ2P in ADF for equilibrium geometries optimized with DFT(M06-L)/SO-ZORA/TZ2P in ADF. Results for PtO_4^{2+}.

Molecule		Bond	r [Å]	MAYER	G-J	**N-M (1)**	N-M (2)	N-M (3)
PtO_4^{2+} (**A**)	M=1	Pt=O	1.711	1.433	1.213	1.208	0.725	0.931
		∑Pt(all)	**-**	**5.734**	**4.854**	**4.831**	**2.902**	**3.723**
	M=3	Pt=O (2x)	1.711	1.471	1.254	1.337	0.910	1.054
		Pt=O (2x)	1.711	1.175	1.025	1.039	0.486	0.785
		∑Pt(all)	**-**	**5.293**	**4.559**	**4.754**	**2.791**	**3.678**
	M=5	Pt=O (3x)	1.711	1.253	1.090	1.126	0.668	0.862
		Pt=O	1.711	1.179	1.034	1.052	0.453	0.783
		∑Pt(all)	**-**	**4.936**	**4.303**	**4.431**	**2.458**	**3.370**
PtO_4^{2+} (**C**)	M=1	Pt=O (1)	1.738	1.676	1.537	1.659	1.262	1.346
		Pt=O (2)	1.739	1.689	1.542	1.667	1.275	1.354
		Pt=O (3)	2.297	0.404	0.314	0.354	-0.059	0.273
		∑Pt(all)	**-**	**3.951**	**3.582**	**3.903**	**1.977**	**3.139**
	M=3	Pt=O (1)	1.738	1.601	1.520	1.586	1.018	1.232
		Pt=O (2)	1.739	1.569	1.468	2.032	1.530	1.701
		Pt=O (3)	2.297	0.374	0.284	0.308	0.110	0.240
		∑Pt(all)	**-**	**3.668**	**3.394**	**4.058**	**2.157**	**3.267**
	M=5	Pt=O (1)	1.738	1.571	1.483	1.589	1.084	1.256
		Pt=O (2)	1.739	1.589	1.498	1.605	1.097	1.269
		Pt=O (3)	2.297	0.382	0.300	0.322	0.093	0.249
		∑Pt(all)	**-**	**3.677**	**3.415**	**3.659**	**1.755**	**2.876**

Table S40. Mulliken spin densities of platinum coordination center and respective ligands for higher multiplicities (M=3,5) for **A**, **C**, **C'** and **C"** structures. Additionally, relative energies with respect to **A** geometry for each system with M=1 are provided. Single-point calculations were carried out both for DFT(M06-L)/ZORA (Orca) and DFT(M06-L)/SO-ZORA (ADF) resulting geometries.

A. Results from single-point calculations DFT(M06-L)/ZORA level of theory with TZ2P basis set in ADF for equilibrium geometries optimized at DFT(M06-L)/ZORA with SARC-ZORA-TZVPP basis set for metal atoms and ZORA-def2-TZVPP for ligands in Orca.

		Spin densities					
Molecule	M	Pt	O	N(1)	N(2)	N(3)	ΔE [kJ/mol]
PtN_3O^- (**A**)	M=1	-	-	-	-	-	0.0
	M=3	-0.153	0.110	0.884	0.883	0.276	+15.8
	M=5	-0.088	0.359	1.312	1.312	1.104	+82.2
PtN_3O^- (**C'**)	M=1	-	-	-	-	-	-294.8
	M=3	-0.133	0.242	0.651	0.651	0.589	-255.1
	M=5	0.082	0.447	1.385	1.385	0.702	-150.5
PtN_3O^- (**C"**)	M=1	-	-	-	-	-	-601.9
	M=3	0.298	0.599	1.018	0.043	0.043	-552.5
	M=5	0.848	1.237	1.690	0.113	0.113	-358.4

		Spin densities					
Molecule	M	Pt	O(1)	O(2)	N(1)	N(2)	ΔE [kJ/mol]
PtN_2O_2 (**A**)	M=1	-	-	-	-	-	0.0
	M=3	0.029	0.057	0.057	0.929	0.929	+74.5
	M=5	0.125	0.626	0.626	1.312	1.311	+188.3
PtN_2O_2 (**C**)	M=1	-	-	-	-	-	-63.3
	M=3	-0.037	-0.126	-0.126	1.144	1.144	+68.7
	M=5	0.299	0.643	0.642	1.208	1.208	+193.2
PtN_2O_2 (**C'**)	M=1	-	-	-	-	-	-208.0
	M=3	0.112	0.284	0.328	0.633	0.644	-206.7
	M=5	0.447	0.860	0.654	1.222	0.816	-44.8
PtN_2O_2 (**C"**)	M=1	-	-	-	-	-	-492.1
	M=3	0.673	0.669	0.669	-0.005	-0.005	-480.4
	M=5	1.383	1.223	1.223	0.085	0.085	-297.0

		Spin densities					
Molecule	M	Pt	O(1)	O(2)	O(3)	N	ΔE [kJ/mol]
$PtNO_3^+$ (**A**)	M=1	-	-	-	-	-	0.0
	M=3	0.233	0.207	0.333	0.364	0.864	+46.3
	M=5	0.534	0.583	0.583	0.925	1.374	+218.2
$PtNO_3^+$ (**C**)	M=1	-	-	-	-	-	-43.8
	M=3	0.348	0.405	0.394	0.394	0.459	-7.4
	M=5	0.718	0.698	0.700	0.700	1.184	+183.6
$PtNO_3^+$ (**C'**)	M=1	-	-	-	-	-	-190.0
	M=3	0.455	0.469	0.469	0.321	0.285	-197.4
	M=5	0.991	0.941	0.941	0.516	0.610	-77.1

Molecule	M	Spin densities					ΔE [kJ/mol]
		Pt	O(1)	O(2)	O(3)	O(4)	
PtO_4^{2+} (**A**)	M=1	-	-	-	-	-	0.0
	M=3	0.039	0.490	0.490	0.490	0.490	+129.1
	M=5	0.164	1.029	1.029	0.889	0.889	+207.9
PtO_4^{2+} (**C**)	M=1	-	-	-	-	-	-130.2
	M=3	0.098	0.455	0.455	0.497	0.497	-137.2
	M=5	0.464	0.958	0.958	0.809	0.809	+9.3

It is clear that for minima (**C**, **C'**) or higher multiplicities of minimum **A** there are substantial spin densities on ligands and/or on central metal cation, which is consistent with much smaller BO values for these states than for the quasi-tetrahedral singlet minimum **A** of interest.

B. Results from single-point calculations DFT(M06-L)/ZORA with TZ2P in ADF for equilibrium geometries optimized with DFT(M06-L)/SO-ZORA with TZ2P in ADF.

		Spin densities					
Molecule	M	Pt	O	N(1)	N(2)	N(3)	ΔE [kJ/mol]
PtN_3O^- (**A**)	M=1	-	-	-	-	-	0.0
	M=3	-0.021	-0.017	0.609	0.610	0.819	+82.7
	M=5	0.079	0.340	1.124	1.124	1.334	+152.2
PtN_3O^- (**C'**)	M=1	-	-	-	-	-	-314.5
	M=3	0.026	0.620	-0.458	0.870	0.942	-263.4
	M=5	0.326	0.666	0.874	1.138	0.996	-134.6
PtN_3O^- (**C''**)	M=1	-	-	-	-	-	-700.2
	M=3	0.589	0.244	1.167	0.000	0.000	-491.8
	M=5	1.071	0.978	1.938	0.007	0.007	-286.1

		Spin densities					
Molecule	M	Pt	O(1)	O(2)	N(1)	N(2)	ΔE [kJ/mol]
PtN_2O_2 (**A**)	M=1	-	-	-	-	-	0.0
	M=3	0.028	0.053	0.053	0.933	0.933	+73.3
	M=5	0.122	0.629	0.629	1.310	1.310	+184.6
PtN_2O_2 (**C**)	M=1	-	-	-	-	-	-68.3
	M=3	-0.044	-0.127	-0.127	1.148	1.148	+61.2
	M=5	0.295	0.641	0.641	1.212	1.211	+187.1
PtN_2O_2 (**C'**)	M=1	-	-	-	-	-	-401.7
	M=3	0.312	0.405	0.521	0.044	0.718	-297.3
	M=5	0.582	0.920	0.520	1.234	0.744	-94.1
PtN_2O_2 (**C''**)	M=1	-	-	-	-	-	-708.5
	M=3	1.265	0.368	0.368	0.000	0.000	-562.2
	M=5	1.690	1.155	1.155	0.000	0.000	-356.6

		Spin densities					
Molecule	M	Pt	O(1)	O(2)	O(3)	N	ΔE [kJ/mol]
$PtNO_3^+$ (**A**)	M=1	-	-	-	-	-	0.0
	M=3	0.092	0.728	0.728	-0.287	0.738	+133.8
	M=5	0.200	0.768	0.768	0.768	1.497	+183.5
$PtNO_3^+$ (**C**)	M=1	-	-	-	-	-	-105.7
	M=3	0.306	0.743	0.689	0.689	-0.427	-55.6
	M=5	0.388	0.988	0.758	0.758	1.109	+129.0
$PtNO_3^+$ (**C'**)	M=1	-	-	-	-	-	-470.7
	M=3	0.510	0.723	0.229	0.273	0.265	-387.4
	M=5	0.964	1.296	1.162	0.304	0.275	-258.1

		Spin densities					
Molecule	M	Pt	O(1)	O(2)	O(3)	O(4)	ΔE [kJ/mol]
PtO_4^{2+} (**A**)	M=1	-	-	-	-	-	0.0
	M=3	0.203	-0.189	-0.189	1.087	1.087	+114.4
	M=5	0.156	0.895	0.895	1.159	0.895	+203.7
PtO_4^{2+} (**C**)	M=1	-	-	-	-	-	-161.3
	M=3	0.182	1.200	-1.021	1.086	0.553	-292.2
	M=5	0.571	0.917	0.910	1.071	0.532	-272.8

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Appendix S1. Cartesian coordinates [Å] (XYZ format) of minimum energy and transition state equilibrium structures discussed in the text. Equilibrium geometries were mostly obtained from DFT(M06-L)/ZORA calculations. In a few cases, when this approach gave no positive result, DFT(B3LYP)/ZORA method was used (indicated in red). All equilibrium structures were optimized as single spin multiplicity. Some structures are quoted from our previous work[1].

```
5
Structure OsO4 A - DFT(M06-L)/ZORA, Ref[1]
  O      0.000000    0.000033    1.698203
  Os     0.000000   -0.000026   -0.000065
  O     -0.000000   -1.601234   -0.566072
  O      1.386682    0.800613   -0.566034
  O     -1.386682    0.800614   -0.566034

5
Structure OsO4 B - DFT(M06-L)/ZORA, Ref[1]
  Os    -0.125014   -0.071711   -0.235124
  O      0.421197    0.239939    1.604417
  O     -0.108520   -1.711470   -0.655188
  O      1.351340    0.781577   -0.064595
  O     -1.539000    0.761664   -0.649510

5
Structure OsO4 C - DFT(M06-L)/ZORA, Ref[1]
  Os    -0.000027   -0.000046    0.121495
  O      0.000010   -0.710292   -1.627900
  O     -1.436736    0.000006    0.996567
  O      0.000208    0.710720   -1.627687
  O      1.436544   -0.000388    0.996793

5
Structure OsO4 D - DFT(M06-L)/ZORA, Ref[1]
  Os    -0.144420   -0.148535   -0.069841
  O     -0.783324    1.398774    0.150366
  O      2.124668    0.616349    0.252052
  O      1.645658   -0.539912   -0.210889
  O     -1.279186   -1.372627   -0.255386

5
Structure OsO4 E - DFT(M06-L)/ZORA, Ref[1]
  Os    -0.187243   -0.022547   -0.022763
  O     -0.961324    1.472451    0.028569
  O      1.604955   -0.301638    0.025873
  O      2.715105    0.305246    0.097060
  O     -1.067953   -1.453512   -0.128737

5
Structure OsNO3- A - DFT(M06-L)/ZORA
  Os    -0.000000    0.000010   -0.017852
  O     -1.431854   -0.826674    0.537546
  O      1.431854   -0.826673    0.537546
  O      0.000000    1.653372    0.537591
  N      0.000000   -0.000034   -1.701807

5
Structure OsNO3- B - DFT(M06-L)/ZORA
  Os     0.039321    0.223663   -0.144415
  O     -0.590338   -1.163160    0.741872
  O      1.391300   -1.041560    0.667110
  O      0.033432    1.860960    0.445689
  N      0.026285    0.120100   -1.817234

5
Structure OsNO3- C - DFT(M06-L)/ZORA
  Os    -0.012626    0.140834    0.000097
  O     -1.327152    1.279416    0.004775
  O     -0.076693   -1.669251   -0.719585
  O     -0.071726   -1.669408    0.719826
  N      1.501789    0.834847   -0.005112

5
Structure OsNO3- D - DFT(M06-L)/ZORA
  Os    -0.172876   -0.087255   -0.051859
  O     -0.983259    1.417036    0.269705
  O      2.335638    0.551351    0.131001
  O      1.613346   -0.585106   -0.133619
  N     -1.229451   -1.341978   -0.348925

5
Structure OsNO3- E - DFT(M06-L)/ZORA
  Os    -0.077191   -0.071293   -0.021220
  O     -0.876867    1.471197    0.032738
  O      1.707493   -0.582483    0.014145
  O      2.482058    0.539840    0.101305
  N     -1.131953   -1.357262   -0.126969

5
Structure OsNO3- B' - DFT(M06-L)/ZORA
  Os     0.000331   -0.223034    0.102209
  O     -1.478991   -0.965504    0.624559
  O      1.483342   -0.971389    0.605280
  O      0.003833    1.711240    0.037884
  N     -0.008517    0.448687   -1.476908

5
Structure OsNO3- C' - DFT(M06-L)/ZORA
  Os    -0.059660   -0.067196    0.000000
  O      0.022278   -0.988821   -1.457514
  O      0.022279   -0.988820    1.457514
  O     -0.622459    1.768403    0.000001
  N      0.761088    1.583218   -0.000001

5
Structure OsNO3- D' - DFT(M06-L)/ZORA
  Os     0.213974    0.099859   -0.323128
  O      0.047326    1.525897    0.650727
  O     -0.243668   -1.480408    0.182456
  O      0.885618   -0.554830   -2.283415
  N     -0.085886    0.348437   -2.122949

5
Structure OsNO3- E' - DFT(M06-L)/ZORA
  Os    -0.009296    0.011628   -0.297947
  O      0.134333    1.586906    0.434878
  O     -0.172665   -1.535400    0.488979
  O      0.032640   -0.042879   -3.239975
  N      0.014987   -0.020253   -2.025526

5
Structure IrO4+ A - DFT(M06-L)/ZORA
  Ir     0.000000    0.000041   -0.021295
  O     -1.377486   -0.795335    0.540851
  O      1.377484   -0.795334    0.540858
  O     -0.000000    1.590667    0.540889
  O      0.000003   -0.000038   -1.708280

5
Structure IrO4+ B - DFT(B3LYP)/ZORA
  Ir     0.010035    0.165333   -0.136988
  O     -0.674187   -1.105401    0.769446
  O      1.404508   -0.889402    0.597196
  O      0.090141    1.728735    0.481123
  O      0.069503    0.100737   -1.817755

5
Structure IrO4+ C - DFT(M06-L)/ZORA
  Ir     0.012660   -0.089624    0.000001
  O     -0.018141   -0.957489   -1.424984
  O     -0.018140   -0.957489    1.424985
  O     -0.616147    1.679786    0.000000
  O      0.763292    1.631601    0.000000
```

```
5
Structure IrO4+ D - DFT(M06-L)/ZORA
  Ir    -0.158400   -0.128777   -0.033803
  O     -0.658911    1.464467    0.037613
  O      1.905109    0.420499    0.508521
  O      1.649955   -0.349059   -0.523445
  O     -1.174355   -1.453079   -0.122586

5
Structure IrO4+ E - DFT(M06-L)/ZORA
  Ir    -0.234115   -0.019918   -0.023967
  O     -0.885445    1.513655    0.034925
  O      1.650105   -0.370975    0.023295
  O      2.613025    0.356262    0.095417
  O     -1.040030   -1.479026   -0.129669

5
Structure IrNO3 A - DFT(M06-L)/ZORA, Ref[1]
  Ir    -0.000000    0.000058   -0.012087
  O     -1.415043   -0.817058    0.530436
  O      1.415043   -0.817057    0.530436
  O      0.000001    1.634107    0.530485
  N      0.000000   -0.000049   -1.686248

5
Structure IrNO3 B - DFT(M06-L)/ZORA, Ref[1]
  Ir     0.029245    0.184766   -0.125182
  O     -0.677709   -1.124778    0.782118
  O      1.426871   -0.966446    0.566694
  O      0.035540    1.801121    0.458460
  N      0.086054    0.105340   -1.789068

5
Structure IrNO3 C - DFT(M06-L)/ZORA, Ref[1]
  Ir    -0.016938    0.136249    0.000113
  O     -1.313039    1.258892    0.004725
  O     -0.074209   -1.647673   -0.703935
  O     -0.069365   -1.647832    0.704164
  N      1.487143    0.816802   -0.005066

5
Structure IrNO3 D - DFT(M06-L)/ZORA, Ref[1]
  Ir    -0.072572   -0.062761   -0.057532
  O     -0.882005    1.449047    0.123085
  O      1.960299    0.511406    0.371067
  O      1.690725   -0.609145   -0.389780
  N     -1.133050   -1.334498   -0.180538

5
Structure IrNO3 E - DFT(M06-L)/ZORA, Ref[1]
  Ir    -0.154446   -0.021237   -0.021421
  O     -0.974472    1.488055    0.030420
  O      1.686065   -0.466193    0.019522
  O      2.610028    0.396907    0.098057
  N     -1.063635   -1.397533   -0.126579

5
Structure IrNO3 B' - DFT(M06-L)/ZORA, Ref[1]
  Ir     0.000001   -0.200823    0.074356
  O     -1.459679   -0.927133    0.602936
  O      1.459680   -0.927134    0.602937
  O     -0.000001    1.677351    0.133205
  N     -0.000000    0.377739   -1.520409

5
Structure IrNO3 C' - DFT(M06-L)/ZORA, Ref[1]
  Ir    -0.073711   -0.075406   -0.000001
  O      0.028755   -1.000250   -1.429450
  O      0.028756   -1.000248    1.429450
  O     -0.580815    1.785258    0.000001
  N      0.720542    1.597430   -0.000000

5
Structure IrNO3 D' - DFT(M06-L)/ZORA, Ref[1]
  Ir     0.265487    0.098623   -0.278360
  O      0.047402    1.520837    0.657644
  O     -0.300298   -1.451792    0.187848
  O      0.892895   -0.472220   -2.341096
  N     -0.088124    0.243507   -2.122346

5
Structure IrNO3 E' - DFT(M06-L)/ZORA, Ref[1]
  Ir    -0.014982   -0.049273   -0.281344
  O      0.121547    1.540878    0.360263
  O     -0.166815   -1.566293    0.491753
  O      0.022647   -0.141113   -3.160659
  N      0.037602    0.215804   -2.049603

5
Structure IrN2O2- A - DFT(M06-L)/ZORA
  Ir    -0.730041    0.260616   -0.161472
  O     -0.135230    1.077960    1.289655
  O     -0.160676    1.092504   -1.614535
  N     -0.166695   -1.348937   -0.174455
  N     -2.435322    0.252469   -0.146650

5
Structure IrN2O2- B - DFT(M06-L)/ZORA
  Ir    -0.586303    0.018669    0.249472
  O     -2.207634    0.373566   -0.397762
  O     -0.466516    1.014163   -1.490144
  N      0.111750   -1.527722    0.118177
  N      0.089861    0.926238    1.520258

5
Structure IrN2O2- C - DFT(M06-L)/ZORA
  Ir     0.000099   -0.001917   -0.184526
  O      0.677604    0.005547    1.671996
  O     -0.759580    0.009510    1.640154
  N      0.016853   -1.429421   -1.101089
  N      0.024985    1.416022   -1.115643

5
Structure IrN2O2- D - DFT(M06-L)/ZORA
  Ir    -0.228668    0.530576    0.026863
  O     -0.436908   -1.351345   -0.232905
  O     -1.725716   -1.527785    0.202590
  N     -1.433210    1.695908   -0.268746
  N      1.336453    1.176355    0.161739

5
Structure IrN2O2- E - DFT(M06-L)/ZORA
  Ir    -0.167182   -0.060289   -0.023836
  O      1.698568   -0.400605    0.023303
  O      2.718269    0.431211    0.103752
  N     -1.195334   -1.414623   -0.132166
  N     -0.950782    1.444304    0.028947

5
Structure IrN2O2- B' - DFT(M06-L)/ZORA
  Ir    -0.646128    0.158454    0.025890
  O     -0.080990    0.933133    1.502338
  O     -0.517064    1.186629   -1.615319
  N     -0.137869   -1.445666   -0.180568
  N     -2.245914    0.502064   -0.539798

5
Structure IrN2O2- C' - DFT(M06-L)/ZORA
  Ir     0.014816    0.127446    0.073596
  O     -1.337717    1.249591   -0.047931
  O     -0.068286   -1.740407    0.680743
  N      1.523036    0.867938   -0.031086
  N     -0.118256   -1.588128   -0.675320

5
Structure IrN2O2- D' - DFT(M06-L)/ZORA
  Ir    -0.724690    0.027367    0.944118
  O     -2.124833    0.528914    1.893871
  O     -1.334915   -1.694946   -1.262348
  N     -0.931575   -1.790421   -0.151303
  N      0.860908    0.457164    0.582361

5
Structure IrN2O2- E' - DFT(M06-L)/ZORA
  Ir    -0.438983   -0.344643   -0.008791
  O      1.666381    1.469502    0.031807
```

```
  O      0.344271   -1.880352   -0.330200
  N     -2.074304   -0.034239    0.221170
  N      0.457895    1.336283    0.146269

5
Structure IrN2O2- B" - DFT(B3LYP)/ZORA
  Ir    -0.606392    0.052900    0.189220
  O      0.086973   -1.565992    0.075269
  O      0.063964    0.982108    1.531511
  N     -2.192382    0.334300   -0.328338
  N     -0.411005    1.001599   -1.467661

5
Structure IrN2O2- C" - DFT(M06-L)/ZORA
  Ir     0.015687   -0.078602   -0.000000
  O     -0.010202   -1.064592   -1.450265
  O     -0.010194   -1.064591    1.450266
  N     -0.555372    1.773723   -0.000008
  N      0.683608    1.740846    0.000008

5
Structure IrN2O2- D" - DFT(M06-L)/ZORA
  Ir    -0.432046   -0.464168    0.598240
  O     -0.292777   -2.199379    0.187863
  O      0.482035    0.347439    1.822228
  N     -2.423773   -0.824006   -0.306476
  N     -1.934858    0.135303   -0.747472

5
Structure IrN2O2- E" - DFT(M06-L)/ZORA
  Ir    -0.263311    0.188013   -0.189308
  N      1.567306   -0.154156   -0.010368
  N      2.692681   -0.125481    0.158828
  O     -0.681353   -1.543355   -0.018309
  O     -1.211783    1.634977    0.059159

5
Structure PtNO3+ A - DFT(M06-L)/ZORA
  Pt     0.000000    0.000061   -0.008240
  O     -1.419904   -0.819856    0.535873
  O      1.419904   -0.819856    0.535874
  O     -0.000000    1.639710    0.535935
  N     -0.000000   -0.000059   -1.706419

5
Structure PtNO3+ B - DFT(B3LYP)/ZORA
  Pt    -0.021719    0.145455   -0.109088
  O     -0.844472   -1.088104    0.798084
  O      1.570703   -0.879317    0.490923
  O      0.063398    1.759345    0.502703
  N      0.132091    0.062624   -1.789599

5
Structure PtNO3+ C - DFT(M06-L)/ZORA
  Pt    -0.021104    0.144159    0.000046
  O     -1.308472    1.280943    0.004743
  O     -0.077511   -1.678036   -0.675361
  O     -0.072832   -1.678117    0.675617
  N      1.493512    0.847490   -0.005044

5
Structure PtNO3+ D - DFT(M06-L)/ZORA
  Pt    -0.114807    0.265408   -0.042243
  O     -1.185462    1.602437    0.005387
  O      1.745049    0.035357    0.482614
  O      1.835657   -0.642126   -0.609675
  N     -0.717040   -1.307027    0.030220

5
Structure PtNO3+ E - DFT(M06-L)/ZORA
  Pt    -0.241159    0.013960   -0.022885
  O     -1.007674    1.552735    0.031822
  O      1.749621   -0.461934    0.022734
  O      2.628071    0.350895    0.097066
  N     -1.025319   -1.455657   -0.128737

5
Structure PtNO3+ B' - DFT(M06-L)/ZORA
  Pt    -0.000000   -0.183430    0.048770
  O     -1.453424   -0.906796    0.612276
  O      1.453424   -0.906795    0.612279
  O      0.000001    1.667710    0.212243
  N     -0.000001    0.329311   -1.592544

5
Structure PtNO3+ C' - DFT(M06-L)/ZORA
  Pt    -0.113467   -0.125598    0.000000
  O      0.048978   -1.086796   -1.418614
  O      0.048980   -1.086797    1.418614
  O     -0.514583    1.931090   -0.000002
  N      0.653617    1.674886    0.000001

5
Structure PtNO3+ D' - DFT(M06-L)/ZORA
  Pt     0.297964    0.072044   -0.260648
  O      0.057668    1.477523    0.713139
  O     -0.398168   -1.403677    0.340463
  O      0.954379   -0.313562   -2.474047
  N     -0.094479    0.106627   -2.215217

5
Structure PtNO3+ E' - DFT(M06-L)/ZORA
  Pt    -0.200621   -0.095931   -0.093495
  O     -0.831133    1.408540    0.561017
  O      1.956986    0.201849   -0.538038
  O      1.897116   -0.322975    0.607874
  N     -1.258951   -1.237434   -0.671056

5
Structure PtN2O2 A - DFT(M06-L)/ZORA
  Pt    -0.728007    0.263451   -0.161463
  O     -0.136982    1.075575    1.287341
  O     -0.162404    1.090073   -1.612200
  N     -0.157262   -1.354142   -0.174577
  N     -2.443308    0.259655   -0.146557

5
Structure PtN2O2 B - DFT(M06-L)/ZORA
  Pt     0.001866    0.149772   -0.135334
  O     -0.774520   -1.081836    0.890145
  O      1.492903   -0.934046    0.494395
  N      0.014057    1.739906    0.489247
  N      0.165695    0.126207   -1.845430

5
Structure PtN2O2 C - DFT(M06-L)/ZORA
  Pt    -0.000244   -0.001907   -0.184848
  O      0.658345    0.005584    1.672109
  O     -0.740275    0.009467    1.641312
  N      0.016993   -1.434837   -1.101527
  N      0.025143    1.421434   -1.116153

5
Structure PtN2O2 D - DFT(M06-L)/ZORA
  Pt    -0.183843    0.517400   -0.059457
  O     -0.569329   -1.340583    0.443767
  O     -1.605806   -1.426452   -0.348939
  N     -1.514292    1.606412    0.017871
  N      1.385220    1.166933   -0.163699

5
Structure PtN2O2 E - DFT(M06-L)/ZORA
  Pt    -0.196957   -0.042991   -0.023844
  O      1.740665   -0.416898    0.024159
  O      2.667365    0.420286    0.101133
  N     -1.169363   -1.451027   -0.133127
  N     -0.938170    1.490629    0.031680

5
Structure PtN2O2 B' - DFT(M06-L)/ZORA
  Pt    -0.831188    0.294158    0.005005
  O     -0.220622    1.029340    1.475125
  O      0.056984    0.805580   -1.592373
  N     -0.112029   -1.202449   -0.521094
  N     -2.521110    0.407984   -0.174120
```

```
5
Structure PtN2O2 C' - DFT(M06-L)/ZORA
  Pt     0.020660    0.153568    0.091624
  O     -1.321519    1.286346   -0.068783
  O     -0.065797   -1.823972    0.628655
  N      1.524641    0.931708   -0.035617
  N     -0.144392   -1.631211   -0.615878

5
Structure PtN2O2 D' - DFT(M06-L)/ZORA
  Pt    -0.285899    0.480705   -0.166923
  N     -0.708102   -1.254221    0.589294
  O     -1.332406   -1.449800   -0.453725
  N     -1.520213    1.631730    0.117917
  O      1.358570    1.115295   -0.197021

5
Structure PtN2O2 E' - DFT(M06-L)/ZORA
  Pt    -0.561994   -0.485120   -0.016979
  O      1.640975    1.380817    0.022357
  O      0.503380   -1.832668   -0.340358
  N     -2.132440    0.060718    0.240714
  N      0.505339    1.422803    0.154521

5
Structure PtN2O2 B" - DFT(M06-L)/ZORA(B3LYP)
  Pt    -0.633628    0.054814    0.185419
  O      0.094012   -1.541568    0.064373
  O      0.071241    0.979187    1.504978
  N     -2.250162    0.311462   -0.289258
  N     -0.340304    1.001020   -1.465510

5
Structure PtN2O2 C" - DFT(M06-L)/ZORA
  Pt     0.013901   -0.148359    0.000001
  O     -0.011931   -1.128621   -1.448815
  O     -0.011929   -1.128620    1.448815
  N     -0.511393    1.871474   -0.000001
  N      0.644878    1.840911    0.000001

5
Structure PtN2O2 D" - DFT(M06-L)/ZORA
  Pt    -0.468798   -0.495023    0.579894
  O     -0.096049   -2.194856    0.225926
  O      0.456400    0.240336    1.848299
  N     -2.512281   -0.628306   -0.190332
  N     -1.980693    0.073038   -0.909404

5
Structure PtN2O2 E" - DFT(M06-L)/ZORA
  Pt    -0.032946   -0.060446    0.890416
  O      0.129239    1.629030    0.865375
  O     -0.194416   -1.750425    0.899725
  N      0.050441   -0.272801   -4.056574
  N      0.047680    0.454642   -3.238532

5
Structure PtN3O- A - DFT(M06-L)/ZORA
  Pt    -0.000000    0.000050    0.008205
  N     -1.433251   -0.827594    0.563299
  N      1.433251   -0.827593    0.563299
  N      0.000000    1.655137    0.563285
  O     -0.000000    0.000001   -1.805065

5
Structure PtN3O- B' - DFT(M06-L)/ZORA
  Pt    -0.000002   -0.116223    0.165378
  N     -1.457066   -0.942268    0.621000
  N      1.457067   -0.942258    0.621000
  N      0.000001    1.650150    0.222937
  O     -0.000000    0.350599   -1.737290

5
Structure PtN3O- C' - DFT(M06-L)/ZORA
  Pt     0.072853   -0.117143   -0.000000
  N     -0.058885   -1.049643   -1.461368
  N     -0.058885   -1.049643    1.461369
  N     -0.577766    1.699199    0.000001
  O      0.746209    1.824014   -0.000001

5
Structure PtN3O- D' - DFT(M06-L)/ZORA
  Pt     0.177633    0.045986   -0.337979
  N      0.132711    1.474659    0.656722
  N     -0.350451   -1.463818    0.369754
  O      1.014103   -0.327314   -2.355465
  N     -0.156633    0.209442   -2.229342

5
Structure PtN3O- E' - DFT(M06-L)/ZORA
  Pt    -0.007512    0.034489   -0.251051
  N      0.120660    1.561324    0.567352
  N     -0.165869   -1.576363    0.343926
  O     -0.006235   -0.433509   -3.071552
  N      0.058958    0.414060   -2.228265

5
Structure PtN3O- B" - DFT(B3LYP)/ZORA
  Pt     0.040958    0.140858   -0.091187
  N     -0.815569   -1.150058    0.713126
  N      1.551993   -0.827864    0.664697
  N      0.153827    1.755556    0.508631
  O     -0.031207    0.081511   -1.902246

5
Structure PtN3O- C" - DFT(M06-L)/ZORA
  Pt     0.014259    0.176760    0.000058
  N     -1.311219    1.287965    0.004712
  N     -0.151463   -1.805239   -0.593237
  N     -0.147466   -1.805412    0.593964
  O      1.609483    1.062365   -0.005497

5
Structure PtN3O- D" - DFT(M06-L)/ZORA
  Pt    -0.094568    0.110736    0.050009
  N     -1.074114    1.524352   -0.025837
  N      1.960757   -0.019473    0.513622
  N      1.856701   -0.227556   -0.643098
  O     -1.085378   -1.434009   -0.028393

5
Structure PtN3O- E" - DFT(M06-L)/ZORA
  Pt    -1.096530   -0.144426   -0.080188
  N     -0.330609    1.370426    0.022368
  N      2.557654   -0.267924    0.089635
  N      2.806902    0.797127    0.153889
  O     -1.833877   -1.755204   -0.185704

5
Structure AuO2N2+ A - DFT(M06-L)/ZORA
 Au     0.001317    0.000745   -0.020190
  O    -1.456471   -0.840842    0.595199
  N     1.442041   -0.840556    0.565127
  N    -0.006973    1.669011    0.565311
  O     0.020086    0.011643   -1.812425

5
Structure AuO2N2+ C - DFT(M06-L)/ZORA
 Au     0.011351   -0.141449   -0.000013
  N    -0.019718   -1.088518   -1.479144
  N    -0.019718   -1.088545    1.479106
  O    -0.579807    1.834507    0.000011
  O     0.731417    1.790790    0.000041

5
Structure AuO2N2+ D - DFT(M06-L)/ZORA
 Au     0.090618    0.407459   -0.152620
  N     0.065131    1.621368    1.085452
  N    -0.109212   -1.400880   -0.135802
  O     0.801770   -0.781653   -2.327271
  O    -0.030943    0.092659   -2.366069

5
Structure AuO2N2+ E - DFT(M06-L)/ZORA
 Au    -0.012126   -0.001063   -0.162176
  N     0.120992    1.582709    0.609815
```

```
  N    -0.171591    -1.619912     0.493139
  O     0.000041    -0.386947    -3.219849
  O     0.062682     0.425211    -2.360518

5
Structure AuO2N2+ B' - DFT(M06-L)/ZORA
 Au    -0.009424    -0.097704     0.120874
  O    -1.483670    -0.939440     0.659212
  N     1.459118    -0.926643     0.600421
  N    -0.010932     1.695624     0.253937
  O     0.044907     0.268163    -1.74142

5
Structure AuO2N2+ C" - DFT(M06-L)/ZORA
 Au     0.053404     0.384713    -0.000180
  O    -1.382825     1.442287     0.004987
  N    -0.151762    -2.052123    -0.553406
  N    -0.147940    -2.052614     0.554199
  O     1.642716     1.194176    -0.005600

5
Structure AuN3O A - DFT(M06-L)/ZORA
 Au     0.000069     0.000065     0.012532
  N    -1.466271    -0.846717     0.566103
  N     1.466307    -0.846753     0.566198
  N     0.000079     1.693329     0.566289
  O    -0.000184     0.000076    -1.818099

5
Structure AuN3O B' - DFT(M06-L)/ZORA
 Au    -0.000040    -0.082800     0.147026
  N    -1.479428    -0.935741     0.616369
  N     1.479054    -0.935815     0.617137
  N     0.000026     1.716008     0.274735
  O     0.000388     0.238349    -1.762243

5
Structure AuN3O E' - DFT(M06-L)/ZORA
 Au    -0.082724    -0.688368     0.000540
  N    -0.058112    -0.995094    -1.741507
  N    -0.061691    -0.992634     1.743107
  N    -0.311026     1.688041    -0.000399
  O     0.637078     2.294841    -0.001740

5
Structure AuN3O B" - DFT(M06-L)/ZORA
 Au     0.246716     0.142562    -0.124040
  O    -0.928266    -1.102881     0.779743
  N     1.568805    -0.863162     0.577539
  N     0.022349     1.771492     0.533841
  N    -0.009605     0.051991    -1.874060

5
Structure AuN4- A - DFT(M06-L)/ZORA
  N     0.000003    -0.000012     1.812915
 Au    -0.000000     0.000011     0.000025
  N    -0.000003    -1.709044    -0.604305
  N     1.480137     0.854524    -0.604316
  N    -1.480137     0.854522    -0.604320

5
Structure AuN4- B" - DFT(M06-L)/ZORA
 Au    -0.118185    -0.064156    -0.238104
  N     0.285314     0.168331     1.747692
  N    -0.029538    -1.805843    -0.632815
  N     1.454878     0.828827    -0.256939
  N    -1.592466     0.872841    -0.619833

5
Structure HgN4 A - DFT(M06-L)/ZORA
  N     0.000000     0.000025     1.888744
 Hg    -0.000000    -0.000063    -0.000130
  N    -0.000000    -1.781111    -0.629547
  N     1.542351     0.890574    -0.629535
  N    -1.542351     0.890576    -0.629534

5
Structure HgN4 B" - DFT(M06-L)/ZORA
 Hg    -0.035340    -0.019947    -0.237977
  N     0.118630     0.064377     1.888568
  N    -0.050017    -1.813891    -0.604379
  N     1.565014     0.906153    -0.448093
  N    -1.598283     0.863307    -0.598119
```

Appendix S2. Cartesian coordinates [Å] (XYZ format) of DFT/ZORA relaxed surface scans steps for investigated reactions paths. In description of each structure its chemical formula and interatomic distance between dissociating ligands are indicated. For energies of structures see Tables S11-S17.

```
  5
OsO4 minimum A d(O-O)=2.773
  O      0.000000    0.000033    1.698203
  Os     0.000000   -0.000026   -0.000065
  O     -0.000000   -1.601234   -0.566072
  O      1.386682    0.800613   -0.566034
  O     -1.386682    0.800614   -0.566034

  5
OsO4 d(O-O)=2.740
  O     -0.000099   -1.389327   -1.212013
  Os     0.000000    0.000022   -0.231945
  O     -1.385771   -0.005479    0.749423
  O      0.000265    1.400626   -1.195855
  O      1.385604   -0.005843    0.749658

  5
OsO4 d(O-O)=2.690
  O     -0.000095   -1.364243   -1.225899
  Os    -0.000001   -0.000039   -0.220520
  O     -1.388710   -0.005532    0.757748
  O      0.000264    1.375712   -1.210043
  O      1.388541   -0.005897    0.757983

  5
OsO4 d(O-O)=2.640
  O     -0.000090   -1.339170   -1.239515
  Os    -0.000002   -0.000113   -0.209282
  O     -1.391645   -0.005569    0.765877
  O      0.000261    1.350785   -1.223925
  O      1.391475   -0.005934    0.766113

  5
OsO4 d(O-O)=2.540
  O     -0.000086   -1.314090   -1.252846
  Os    -0.000003   -0.000176   -0.198257
  O     -1.394537   -0.005617    0.773843
  O      0.000259    1.325865   -1.237552
  O      1.394365   -0.005983    0.774079

  5
OsO4 d(O-O)=2.490
  O     -0.000082   -1.289005   -1.265862
  Os    -0.000004   -0.000221   -0.187456
  O     -1.397387   -0.005679    0.781623
  O      0.000257    1.300952   -1.250898
  O      1.397214   -0.006046    0.781860

  5
OsO4 d(O-O)=2.540
  O     -0.000077   -1.263932   -1.278580
  Os    -0.000004   -0.000283   -0.176884
  O     -1.400201   -0.005721    0.789198
  O      0.000255    1.276026   -1.263901
  O      1.400027   -0.006089    0.789435

  5
OsO4 d(O-O)=2.490
  O     -0.000073   -1.238873   -1.291071
  Os    -0.000005   -0.000374   -0.166588
  O     -1.402896   -0.005735    0.796651
  O      0.000253    1.251085   -1.276614
  O      1.402721   -0.006103    0.796889

  5
OsO4 d(O-O)=2.440
  O     -0.000069   -1.213807   -1.303311
  Os    -0.000006   -0.000445   -0.156590
  O     -1.405433   -0.005765    0.804022
  O      0.000250    1.226151   -1.289115
  O      1.405256   -0.006134    0.804261

  5
OsO4 d(O-O)=2.390
  O     -0.000064   -1.188737   -1.315253
  Os    -0.000007   -0.000495   -0.146876
  O     -1.407846   -0.005811    0.811258
  O      0.000248    1.201223   -1.301358
  O      1.407669   -0.006181    0.811497

  5
OsO4 d(O-O)=2.340
  O     -0.000060   -1.163655   -1.326852
  Os    -0.000008   -0.000513   -0.137434
  O     -1.410167   -0.005883    0.818320
  O      0.000245    1.176306   -1.313325
  O      1.409988   -0.006254    0.818560

  5
OsO4 d(O-O)=2.290
  O     -0.000056   -1.138579   -1.338154
  Os    -0.000008   -0.000541   -0.128260
  O     -1.412395   -0.005946    0.825207
  O      0.000243    1.151383   -1.324972
  O      1.412215   -0.006317    0.825447

  5
OsO4 d(O-O)=2.240
  O     -0.000052   -1.113519   -1.349248
  Os    -0.000009   -0.000606   -0.119376
  O     -1.414470   -0.005974    0.831989
  O      0.000241    1.126444   -1.336327
  O      1.414289   -0.006346    0.832229

  5
OsO4 d(O-O)=2.190
  O     -0.000048   -1.088459   -1.360123
  Os    -0.000010   -0.000664   -0.110796
  O     -1.416358   -0.006005    0.838708
  O      0.000239    1.101505   -1.347471
  O      1.416176   -0.006377    0.838949

  5
OsO4 d(O-O)=2.140
  O     -0.000043   -1.063396   -1.370766
  Os    -0.000011   -0.000710   -0.102507
  O     -1.418061   -0.006044    0.845352
  O      0.000236    1.076568   -1.358404
  O      1.417878   -0.006417    0.845593

  5
OsO4 d(O-O)=2.090
  O     -0.000039   -1.038335   -1.381195
  Os    -0.000011   -0.000757   -0.094508
  O     -1.419602   -0.006082    0.851927
  O      0.000234    1.051630   -1.369124
  O      1.419417   -0.006456    0.852168

  5
OsO4 d(O-O)=2.040
  O     -0.000035   -1.013279   -1.391283
  Os    -0.000012   -0.000848   -0.086681
  O     -1.421151   -0.006092    0.858219
  O      0.000231    1.026686   -1.379448
  O      1.420966   -0.006467    0.858461

  5
OsO4 TS B d(O-O)=1.986
  Os    -0.125014   -0.071711   -0.235124
  O      0.421197    0.239939    1.604417
```

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  O     -0.108520   -1.711470   -0.655188
  O      1.351340    0.781577   -0.064595
  O     -1.539000    0.761664   -0.649510

  5
OsO4 d(O-O)=1.940
  O     -0.000028   -0.969801   -1.567843
  Os    -0.000025   -0.000036    0.090966
  O     -1.445461    0.000018    0.951720
  O      0.000237    0.970199   -1.567522
  O      1.445277   -0.000381    0.951947

  5
OsO4 d(O-O)=1.890
  O     -0.000025   -0.944795   -1.574016
  Os    -0.000025   -0.000047    0.094242
  O     -1.444612    0.000018    0.956267
  O      0.000235    0.945205   -1.573718
  O      1.444427   -0.000380    0.956493

  5
OsO4 d(O-O)=1.840
  O     -0.000021   -0.919794   -1.580000
  Os    -0.000026   -0.000050    0.097401
  O     -1.443786    0.000017    0.960677
  O      0.000232    0.920206   -1.579713
  O      1.443600   -0.000380    0.960903

  5
OsO4 d(O-O)=1.790
  O     -0.000018   -0.894792   -1.585821
  Os    -0.000026   -0.000050    0.100436
  O     -1.442967    0.000016    0.964985
  O      0.000230    0.895208   -1.585544
  O      1.442780   -0.000381    0.965211

  5
OsO4 d(O-O)=1.740
  O     -0.000014   -0.869791   -1.591536
  Os    -0.000026   -0.000051    0.103391
  O     -1.442139    0.000015    0.969227
  O      0.000227    0.870209   -1.591267
  O      1.441951   -0.000381    0.969453

  5
OsO4 d(O-O)=1.690
  O     -0.000010   -0.844790   -1.597174
  Os    -0.000027   -0.000052    0.106299
  O     -1.441364    0.000014    0.973415
  O      0.000224    0.845210   -1.596913
  O      1.441175   -0.000381    0.973641

  5
OsO4 d(O-O)=1.640
  O     -0.000006   -0.819789   -1.602684
  Os    -0.000027   -0.000053    0.109181
  O     -1.440565    0.000013    0.977488
  O      0.000222    0.820211   -1.602430
  O      1.440375   -0.000382    0.977713

  5
OsO4 d(O-O)=1.590
  O     -0.000002   -0.794788   -1.608196
  Os    -0.000027   -0.000052    0.112097
  O     -1.439959    0.000012    0.981547
  O      0.000219    0.795212   -1.607952
  O      1.439769   -0.000383    0.981772

  5
OsO4 d(O-O)=1.590
  O     -0.000002   -0.794788   -1.608196
  Os    -0.000027   -0.000052    0.112097
  O     -1.439959    0.000012    0.981547
  O      0.000219    0.795212   -1.607952
  O      1.439769   -0.000383    0.981772

  5
OsO4 d(O-O)=1.540
  O      0.000002   -0.769788   -1.613816
  Os    -0.000027   -0.000053    0.114964
  O     -1.439145    0.000011    0.985737
  O      0.000216    0.770212   -1.613579
  O      1.438954   -0.000384    0.985962

  5
OsO4 d(O-O)=1.490
  O      0.000006   -0.744787   -1.619682
  Os    -0.000028   -0.000053    0.117618
  O     -1.438025    0.000010    0.990280
  O      0.000213    0.745213   -1.619453
  O      1.437834   -0.000384    0.990504

  5
OsO4 d(O-O)=1.440
  O      0.000013   -0.694785   -1.631880
  Os    -0.000028   -0.000048    0.123310
  O     -1.435953    0.000006    0.999641
  O      0.000206    0.695215   -1.631670
  O      1.435761   -0.000388    0.999866

  5
OsO4 minimum C d(O-O)=1.421
  Os    -0.000027   -0.000046    0.121495
  O      0.000010   -0.710292   -1.627900
  O     -1.436736    0.000006    0.996567
  O      0.000208    0.710720   -1.627687
  O      1.436544   -0.000388    0.996793

  5
OsNO3- minimum A d(O-O)=2.864
  Os    -0.000000    0.000010   -0.017852
  O     -1.431854   -0.826674    0.537546
  O      1.431854   -0.826673    0.537546
  O      0.000000    1.653372    0.537591
  N      0.000000   -0.000034   -1.701807

  5
OsNO3- d(O-O)=2.840
  Os     0.179608    0.004575   -0.020511
  O     -1.100900   -0.968747    0.646821
  O      1.716070   -0.679055    0.431509
  O      0.052488    1.653294    0.535249
  N      0.052733   -0.010065   -1.700045

  5
OsNO3- d(O-O)=2.790
  Os     0.178238    0.013906   -0.026105
  O     -1.074302   -0.978032    0.652363
  O      1.693079   -0.693501    0.440846
  O      0.051288    1.662396    0.532305
  N      0.051697   -0.004766   -1.706386

  5
OsNO3- d(O-O)=2.740
  Os     0.176888    0.023079   -0.031621
  O     -1.047736   -0.987127    0.657809
  O      1.670056   -0.707757    0.450062
  O      0.050101    1.671345    0.529405
  N      0.050691    0.000462   -1.712633

  5
OsNO3- d(O-O)=2.690
  Os     0.175531    0.032073   -0.037058
  O     -1.021217   -0.996048    0.663165
  O      1.646975   -0.721763    0.459150
  O      0.048979    1.680122    0.526552
  N      0.049731    0.005620   -1.718787

  5
OsNO3- d(O-O)=2.640
  Os     0.174198    0.040881   -0.042407
  O     -0.994731   -1.004738    0.668380
  O      1.623860   -0.735526    0.468114
  O      0.047893    1.688710    0.523765
  N      0.048780    0.010677   -1.724831
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  5
OsNO3- d(O-O)=2.590
  Os     0.172884    0.049493   -0.047665
  O     -0.968284   -1.013198    0.673436
  O      1.600705   -0.749011    0.476959
  O      0.046868    1.697096    0.521051
  N      0.047826    0.015623   -1.730758

  5
OsNO3- d(O-O)=2.540
  Os     0.171592    0.057901   -0.052824
  O     -0.941876   -1.021416    0.678333
  O      1.577508   -0.762220    0.485668
  O      0.045894    1.705275    0.518403
  N      0.046882    0.020462   -1.736557

  5
OsNO3- d(O-O)=2.490
  Os     0.170379    0.066095   -0.057882
  O     -0.915487   -1.029318    0.683103
  O      1.554308   -0.775260    0.494245
  O      0.044856    1.713238    0.515783
  N      0.045944    0.025248   -1.742227

  5
OsNO3- d(O-O)=2.440
  Os     0.169217    0.074053   -0.062824
  O     -0.889120   -1.036987    0.687770
  O      1.531091   -0.788126    0.502716
  O      0.043798    1.721007    0.513116
  N      0.045013    0.030057   -1.747756

  5
OsNO3- d(O-O)=2.390
  Os     0.168048    0.081774   -0.067645
  O     -0.862797   -1.044513    0.692322
  O      1.507818   -0.800719    0.511079
  O      0.042832    1.728590    0.510404
  N      0.044098    0.034872   -1.753138

  5
OsNO3- d(O-O)=2.340
  Os     0.166902    0.089248   -0.072353
  O     -0.836512   -1.051792    0.696756
  O      1.484504   -0.813054    0.519300
  O      0.041894    1.735946    0.507697
  N      0.043212    0.039655   -1.758378

  5
OsNO3- d(O-O)=2.290
  Os     0.165798    0.096482   -0.076963
  O     -0.810259   -1.058794    0.701081
  O      1.461160   -0.825160    0.527389
  O      0.040951    1.743065    0.505001
  N      0.042349    0.044410   -1.763486

  5
OsNO3- d(O-O)=2.240
  Os     0.164733    0.103474   -0.081469
  O     -0.784037   -1.065571    0.705288
  O      1.437787   -0.837039    0.535377
  O      0.040031    1.749964    0.502274
  N      0.041486    0.049175   -1.768448

  5
OsNO3- d(O-O)=2.190
  Os     0.163680    0.110216   -0.085873
  O     -0.757849   -1.072163    0.709399
  O      1.414375   -0.848677    0.543273
  O      0.039160    1.756650    0.499493
  N      0.040633    0.053977   -1.773269

  5
OsNO3- d(O-O)=2.140
  Os     0.162666    0.116717   -0.090184
  O     -0.731686   -1.078531    0.713415
  O      1.390940   -0.860117    0.551074
  O      0.038295    1.763123    0.496666
  N      0.039786    0.058812   -1.777949

  5
OsNO3- d(O-O)=2.090
  Os     0.161730    0.123016   -0.094394
  O     -0.705544   -1.084667    0.717288
  O      1.367498   -0.871416    0.558785
  O      0.037401    1.769428    0.493803
  N      0.038915    0.063642   -1.782460

  5
OsNO3- d(O-O)=2.040
  Os     0.160923    0.129129   -0.098293
  O     -0.679461   -1.090904    0.720806
  O      1.343983   -0.882483    0.566413
  O      0.036640    1.775707    0.490594
  N      0.037915    0.068554   -1.786498

  5
OsNO3- d(O-O)=1.990
  Os     0.037611    0.221286   -0.143251
  O     -0.592841   -1.162678    0.742093
  O      1.391655   -1.036872    0.664335
  O      0.035409    1.858863    0.446318
  N      0.028166    0.119404   -1.816473

  5
OsNO3- TS B' d(O-O)=1.987
  Os     0.000331   -0.223034    0.102209
  O     -1.478991   -0.965504    0.624559
  O      1.483342   -0.971389    0.605280
  O      0.003833    1.711240    0.037884
  N     -0.008517    0.448687   -1.476908

  5
OsNO3- d(O-O)=1.940
  Os     0.059707    0.246312   -0.153949
  O     -0.560438   -1.168246    0.744631
  O      1.377034   -1.087446    0.687415
  O      0.011416    1.881761    0.437392
  N      0.012281    0.127622   -1.822468

  5
OsNO3- d(O-O)=1.890
  Os     0.076414    0.262308   -0.160482
  O     -0.533551   -1.177925    0.752839
  O      1.354562   -1.115261    0.696251
  O     -0.003315    1.896380    0.429981
  N      0.005890    0.134501   -1.825567

  5
OsNO3- d(O-O)=1.840
  Os     0.092333    0.275407   -0.166065
  O     -0.509743   -1.192458    0.763892
  O      1.328137   -1.131727    0.699806
  O     -0.013256    1.907864    0.423333
  N      0.002528    0.140917   -1.827944

  5
OsNO3- d(O-O)1.790
  Os     0.109716    0.287240   -0.171298
  O     -0.489326   -1.214255    0.778501
  O      1.297207   -1.137110    0.698193
  O     -0.019040    1.917628    0.417455
  N      0.001443    0.146501   -1.829828

  5
OsNO3- d(O-O)=1.740
  Os     0.129499    0.297774   -0.176321
  O     -0.477176   -1.264648    0.805510
  O      1.251492   -1.109354    0.682262
  O     -0.010995    1.926245    0.413114
  N      0.007179    0.149986   -1.831543

  5
OsNO3- d(O-O)=1.690
  Os     0.132454    0.301283   -0.178103
  O     -0.456380   -1.287327    0.817210
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  O      1.216901   -1.096670    0.676213
  O     -0.004562    1.930253    0.410882
  N      0.011586    0.152464   -1.833181

  5
OsNO3- d(O-O)=1.640
  Os     0.132164    0.303948   -0.179298
  O     -0.430987   -1.288619    0.816783
  O      1.192831   -1.103326    0.680836
  O     -0.004909    1.933378    0.408988
  N      0.010902    0.154622   -1.834287

  5
OsNO3- d(O-O)=1.590
  Os     0.131728    0.306524   -0.180453
  O     -0.405595   -1.289796    0.816771
  O      1.168719   -1.110097    0.685067
  O     -0.005380    1.936428    0.406982
  N      0.010529    0.156944   -1.835346

  5
OsNO3- d(O-O)=1.540
  Os     0.131330    0.309187   -0.181636
  O     -0.380212   -1.290960    0.816724
  O      1.144599   -1.116898    0.689235
  O     -0.005887    1.939631    0.405154
  N      0.010170    0.159043   -1.836456

  5
OsNO3- d(O-O)=1.490
  Os     0.130899    0.311880   -0.182813
  O     -0.354833   -1.292118    0.816689
  O      1.120469   -1.123710    0.693305
  O     -0.006406    1.942890    0.403356
  N      0.009870    0.161061   -1.837514

  5
OsNO3- d(O-O)=1.440
  Os     0.130479    0.314640   -0.184008
  O     -0.329440   -1.293409    0.816649
  O      1.096353   -1.130614    0.697433
  O     -0.006934    1.946313    0.401538
  N      0.009543    0.163073   -1.838589

  5
OsNO3- minimum C' d(O-O)=1.439
  Os    -0.059660   -0.067196    0.000000
  O      0.022278   -0.988821   -1.457514
  O      0.022279   -0.988820    1.457514
  O     -0.622459    1.768403    0.000001
  N      0.761088    1.583218   -0.000001

  5
OsNO3- minimum A d(N-O)=2.784
  Os    -0.000000    0.000010   -0.017852
  O     -1.431854   -0.826674    0.537546
  O      1.431854   -0.826673    0.537546
  O      0.000000    1.653372    0.537591
  N      0.000000   -0.000034   -1.701807

  5
OsNO3- d(N-O)=2.770
  Os     0.000033   -0.002064   -0.015883
  O     -1.430495   -0.823675    0.551082
  O      1.434495   -0.829437    0.532470
  O      0.006849    1.654505    0.523692
  N     -0.010884    0.000670   -1.698337

  5
OsNO3- d(N-O)=2.720
  Os     0.000066   -0.009866   -0.008722
  O     -1.433514   -0.830511    0.554828
  O      1.437539   -0.836274    0.536201
  O      0.006672    1.650774    0.495978
  N     -0.010765    0.025877   -1.685262

  5
OsNO3- d(N-O)=2.670
  Os     0.000098   -0.017624   -0.001679
  O     -1.436530   -0.837225    0.558489
  O      1.440577   -0.842994    0.539837
  O      0.006492    1.646931    0.468391
  N     -0.010638    0.050912   -1.672013

  5
OsNO3- d(N-O)=2.570
  Os     0.000150   -0.033033    0.011933
  O     -1.442502   -0.850255    0.565627
  O      1.446583   -0.856039    0.546890
  O      0.006124    1.638829    0.413628
  N     -0.010358    0.100498   -1.645053

  5
OsNO3- d(N-O)=2.520
  Os     0.000176   -0.040701    0.018439
  O     -1.445411   -0.856579    0.569148
  O      1.449510   -0.862374    0.550367
  O      0.005938    1.634561    0.386451
  N     -0.010215    0.125093   -1.631380

  5
OsNO3- d(N-O)=2.470
  Os     0.000199   -0.048345    0.024720
  O     -1.448233   -0.862798    0.572662
  O      1.452350   -0.868613    0.553824
  O      0.005743    1.630181    0.359399
  N     -0.010061    0.149575   -1.617582

  5
OsNO3- d(N-O)=2.420
  Os     0.000225   -0.055997    0.030760
  O     -1.450985   -0.868896    0.576153
  O      1.455125   -0.874737    0.557267
  O      0.005548    1.625692    0.332484
  N     -0.009914    0.173938   -1.603640

  5
OsNO3- d(N-O)=2.370
  Os     0.000252   -0.063709    0.036540
  O     -1.453689   -0.874864    0.579607
  O      1.457855   -0.880723    0.560697
  O      0.005362    1.621115    0.305709
  N     -0.009782    0.198181   -1.589530

  5
OsNO3- d(N-O)=2.320
  Os     0.000274   -0.071600    0.041986
  O     -1.456378   -0.880663    0.583083
  O      1.460569   -0.886534    0.564147
  O      0.005181    1.616442    0.279092
  N     -0.009648    0.222356   -1.575283

  5
OsNO3- d(N-O)=2.270
  Os     0.000291   -0.079785    0.046999
  O     -1.459053   -0.886272    0.586653
  O      1.463269   -0.892148    0.567694
  O      0.005007    1.611656    0.252643
  N     -0.009516    0.246549   -1.560965

  5
OsNO3- d(N-O)=2.220
  Os     0.000307   -0.088438    0.051471
  O     -1.461675   -0.891754    0.590410
  O      1.465924   -0.897627    0.571457
  O      0.004847    1.606910    0.226310
  N     -0.009405    0.270909   -1.546624

  5
OsNO3- d(N-O)=2.170
  Os     0.000315   -0.097905    0.055224
  O     -1.464288   -0.897096    0.594499
  O      1.468572   -0.902969    0.575539
  O      0.004681    1.602354    0.200071
  N     -0.009283    0.295617   -1.532309
```

```
  5
OsNO3- d(N-O)=2.120
  Os     0.000304   -0.108884    0.057963
  O     -1.466989   -0.902279    0.599155
  O      1.471305   -0.908156    0.580137
  O      0.004500    1.598304    0.173867
  N     -0.009122    0.321014   -1.518098

  5
OsNO3- d(N-O)=2.070
  Os     0.000275   -0.123003    0.059215
  O     -1.469936   -0.907508    0.604893
  O      1.474292   -0.913391    0.585798
  O      0.004313    1.595865    0.147338
  N     -0.008946    0.348036   -1.504221

  5
OsNO3- d(N-O)=2.020
  Os     0.000207   -0.146901    0.057400
  O     -1.473107   -0.914433    0.613941
  O      1.477541   -0.920350    0.594738
  O      0.004098    1.600954    0.118345
  N     -0.008741    0.380729   -1.491401

  5
OsNO3- TS B d(N-O)=1.972
  Os     0.039321    0.223663   -0.144415
  O     -0.590338   -1.163160    0.741872
  O      1.391300   -1.041560    0.667110
  O      0.033432    1.860960    0.445689
  N      0.026285    0.120100   -1.817234

  5
OsNO3- d(N-O)=1.970
  Os     0.000338   -0.223520    0.103465
  O     -1.478958   -0.966339    0.624522
  O      1.483305   -0.972220    0.605246
  O      0.003828    1.712117    0.036155
  N     -0.008514    0.449962   -1.476364

  5
OsNO3- d(N-O)=1.920
  Os     0.000482   -0.230010    0.128459
  O     -1.478062   -0.982732    0.624804
  O      1.482346   -0.988548    0.605605
  O      0.003677    1.721648   -0.000858
  N     -0.008446    0.479643   -1.464987

  5
OsNO3- d(N-O)=1.870
  Os     0.000600   -0.232651    0.146563
  O     -1.475888   -0.994174    0.626670
  O      1.480156   -1.000013    0.607485
  O      0.003444    1.718714   -0.031241
  N     -0.008313    0.508123   -1.456454

  5
OsNO3- d(N-O)=1.820
  Os     0.000705   -0.234119    0.160874
  O     -1.473920   -1.002394    0.629197
  O      1.478202   -1.008281    0.610038
  O      0.003211    1.708842   -0.057733
  N     -0.008200    0.535953   -1.449351

  5
OsNO3- d(N-O)=1.770
  Os     0.000795   -0.234753    0.172728
  O     -1.472045   -1.009170    0.631881
  O      1.476350   -1.015096    0.612755
  O      0.002995    1.696186   -0.082412
  N     -0.008097    0.562833   -1.441929

  5
OsNO3- d(N-O)=1.720
  Os     0.000868   -0.234804    0.182718
  O     -1.470067   -1.015516    0.634425
  O      1.474390   -1.021457    0.615339
  O      0.002803    1.683397   -0.106550
  N     -0.007996    0.588381   -1.432907

  5
OsNO3- d(N-O)=1.670
  Os     0.000932   -0.234633    0.191179
  O     -1.468070   -1.021619    0.636767
  O      1.472407   -1.027573    0.617717
  O      0.002613    1.671208   -0.130530
  N     -0.007883    0.612618   -1.422109

  5
OsNO3- d(N-O)=1.620
  Os     0.000982   -0.234414    0.198445
  O     -1.466034   -1.027658    0.638985
  O      1.470378   -1.033608    0.619967
  O      0.002434    1.659852   -0.154557
  N     -0.007762    0.635829   -1.409815

  5
OsNO3- d(N-O)=1.570
  Os     0.001024   -0.234242    0.204834
  O     -1.463902   -1.033818    0.641153
  O      1.468249   -1.039755    0.622167
  O      0.002261    1.649527   -0.178827
  N     -0.007634    0.658288   -1.396303

  5
OsNO3- d(N-O)=1.520
  Os     0.001064   -0.234186    0.210603
  O     -1.461654   -1.040211    0.643355
  O      1.466005   -1.046145    0.624397
  O      0.002077    1.640278   -0.203453
  N     -0.007494    0.680265   -1.381877

  5
OsNO3- d(N-O)=1.470
  Os     0.001092   -0.234279    0.215962
  O     -1.459284   -1.046957    0.645692
  O      1.463632   -1.052863    0.626757
  O      0.001907    1.632029   -0.228486
  N     -0.007350    0.702070   -1.366902

  5
OsNO3- d(N-O)=1.420
  Os     0.001125   -0.234380    0.221063
  O     -1.456408   -1.054485    0.648413
  O      1.460762   -1.060381    0.629510
  O      0.001723    1.625078   -0.254191
  N     -0.007203    0.724168   -1.351771

  5
OsNO3- minimum C d(N-O)=1.396
  Os    -0.012626    0.140834    0.000097
  O     -1.327152    1.279416    0.004775
  O     -0.076693   -1.669251   -0.719585
  O     -0.071726   -1.669408    0.719826
  N      1.501789    0.834847   -0.005112

  5
IrO4+ minimum A d(O-O)=2.755
  Ir     0.000000    0.000041   -0.021295
  O     -1.377486   -0.795335    0.540851
  O      1.377484   -0.795334    0.540858
  O     -0.000000    1.590667    0.540889
  O      0.000003   -0.000038   -1.708280

  5
IrO4+ d(O-O)=2.720
  Ir     0.178974    0.006374   -0.025862
  O     -1.044066   -0.932343    0.649944
  O      1.653853   -0.662078    0.434102
  O      0.065855    1.590804    0.542419
  O      0.045386   -0.002756   -1.707582

  5
IrO4+ d(O-O)=2.670
  Ir     0.177551    0.015365   -0.032236
  O     -1.017471   -0.941354    0.656147
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  O      1.630850   -0.676073    0.444198
  O      0.064751    1.598871    0.538990
  O      0.044320    0.003191   -1.714077

  5
IrO4+ d(O-O)=2.620
  Ir     0.176159    0.024168   -0.038488
  O     -0.990911   -0.950128    0.662173
  O      1.607813   -0.689820    0.454149
  O      0.063683    1.606781    0.535659
  O      0.043257    0.009000   -1.720471

  5
IrO4+ d(O-O)=2.570
  Ir     0.174826    0.032774   -0.044574
  O     -0.964376   -0.958672    0.667993
  O      1.584758   -0.703368    0.463950
  O      0.062618    1.614566    0.532370
  O      0.042176    0.014702   -1.726717

  5
IrO4+ d(O-O)=2.520
  Ir     0.173544    0.041157   -0.050486
  O     -0.937869   -0.967013    0.673650
  O      1.561680   -0.716736    0.473610
  O      0.061552    1.622226    0.529057
  O      0.041095    0.020366   -1.732809

  5
IrO4+ d(O-O)=2.470
  Ir     0.172281    0.049293   -0.056238
  O     -0.911401   -0.975168    0.679163
  O      1.538558   -0.729857    0.483139
  O      0.060541    1.629727    0.525726
  O      0.040023    0.026006   -1.738768

  5
IrO4+ d(O-O)=2.420
  Ir     0.171010    0.057182   -0.061821
  O     -0.884981   -0.983151    0.684546
  O      1.515374   -0.742711    0.492498
  O      0.059598    1.637072    0.522380
  O      0.039001    0.031610   -1.744581

  5
IrO4+ d(O-O)=2.370
  Ir     0.021437    0.181282    0.000160
  O     -0.016334   -0.778289   -1.388518
  O     -0.018094   -0.772720    1.392621
  O     -1.115772    1.386190   -0.002991
  O      1.252287    1.290322   -0.001270

  5
IrO4+ d(O-O)=2.320
  Ir     0.021117    0.172126    0.000177
  O     -0.016690   -0.786022   -1.389804
  O     -0.018451   -0.780447    1.393937
  O     -1.090278    1.397433   -0.002997
  O      1.227826    1.303693   -0.001311

  5
IrO4+ d(O-O)=2.270
  Ir     0.020783    0.163300    0.000186
  O     -0.017023   -0.793723   -1.390910
  O     -0.018781   -0.788127    1.395067
  O     -1.064801    1.408502   -0.002998
  O      1.203346    1.316833   -0.001344

  5
IrO4+ d(O-O)=2.220
  Ir     0.020234    0.154706    0.000093
  O     -0.017391   -0.801293   -1.392110
  O     -0.018826   -0.795499    1.396224
  O     -1.039337    1.419333   -0.003101
  O      1.178845    1.329537   -0.001104

  5
IrO4+ d(O-O)=2.170
  Ir     0.058347    0.118312   -0.021519
  O     -0.014238   -0.878126   -1.381450
  O     -0.032223   -0.832031    1.371272
  O     -1.027460    1.509486    0.026341
  O      1.139099    1.389143    0.005358

  5
IrO4+ TS B d(O-O)=2.123
  Ir     0.010035    0.165333   -0.136988
  O     -0.674187   -1.105401    0.769446
  O      1.404508   -0.889402    0.597196
  O      0.090141    1.728735    0.481123
  O      0.069503    0.100737   -1.817755

  5
IrO4+ d(O-O)=2.070
  Ir     0.014853   -0.046578    0.000000
  O     -0.014941   -0.868456   -1.453988
  O     -0.014940   -0.868455    1.453989
  O     -0.965063    1.582119    0.000001
  O      1.103615    1.508156    0.000000

  5
IrO4+ d(O-O)=2.020
  Ir     0.014105   -0.050014    0.000000
  O     -0.015183   -0.874982   -1.451928
  O     -0.015182   -0.874982    1.451929
  O     -0.939481    1.588968    0.000000
  O      1.079265    1.517795    0.000000

  5
IrO4+ d(O-O)=1.970
  Ir     0.013834   -0.053033    0.000000
  O     -0.015387   -0.881806   -1.449484
  O     -0.015386   -0.881806    1.449485
  O     -0.914159    1.596377    0.000000
  O      1.054621    1.527053    0.000000

  5
IrO4+ d(O-O)=1.920
  Ir     0.013601   -0.056781    0.000000
  O     -0.015527   -0.887401   -1.448078
  O     -0.015526   -0.887401    1.448079
  O     -0.888916    1.603019    0.000000
  O      1.029891    1.535349    0.000000

  5
IrO4+ d(O-O)=1.870
  Ir     0.013409   -0.059602    0.000000
  O     -0.015707   -0.893986   -1.445733
  O     -0.015706   -0.893985    1.445734
  O     -0.863654    1.610182    0.000000
  O      1.005181    1.544175    0.000000

  5
IrO4+ d(O-O)=1.820
  Ir     0.013249   -0.063184    0.000000
  O     -0.015881   -0.899315   -1.444403
  O     -0.015880   -0.899314    1.444404
  O     -0.838414    1.616421    0.000000
  O      0.980451    1.552177   -0.000000

  5
IrO4+ d(O-O)=1.770
  Ir     0.013166   -0.065819    0.000000
  O     -0.016145   -0.905799   -1.442018
  O     -0.016144   -0.905799    1.442019
  O     -0.813128    1.623251    0.000000
  O      0.955775    1.560951    0.000000

  5
IrO4+ d(O-O)=1.720
  Ir     0.013065   -0.069318    0.000000
  O     -0.016351   -0.911090   -1.440673
  O     -0.016350   -0.911089    1.440675
  O     -0.787888    1.629375    0.000000
  O      0.931048    1.568907   -0.000000
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  5
IrO4+ d(O-O)=1.670
  Ir     0.012972   -0.071679    0.000000
  O     -0.016592   -0.917894   -1.437976
  O     -0.016591   -0.917894    1.437977
  O     -0.762617    1.636464    0.000000
  O      0.906352    1.577789   -0.000000

  5
IrO4+ d(O-O)=1.620
  Ir     0.012853   -0.075084    0.000000
  O     -0.016796   -0.923462   -1.436485
  O     -0.016795   -0.923462    1.436486
  O     -0.737370    1.642831    0.000000
  O      0.881632    1.585962   -0.000000

  5
IrO4+ d(O-O)=1.570
  Ir     0.012810   -0.078067    0.000000
  O     -0.017054   -0.929504   -1.434563
  O     -0.017053   -0.929504    1.434564
  O     -0.712108    1.649409    0.000000
  O      0.856929    1.594452    0.000000

  5
IrO4+ d(O-O)=1.520
  Ir     0.012788   -0.080274    0.000000
  O     -0.017345   -0.937137   -1.431294
  O     -0.017344   -0.937136    1.431295
  O     -0.686822    1.657254    0.000000
  O      0.832247    1.604078    0.000000

  5
IrO4+ d(O-O)=1.470
  Ir     0.012765   -0.083954    0.000000
  O     -0.017606   -0.943265   -1.429774
  O     -0.017605   -0.943265    1.429775
  O     -0.661567    1.664314    0.000000
  O      0.807536    1.612956   -0.000000

  5
IrO4+ d(O-O)=1.420
  Ir     0.012623   -0.087053    0.000000
  O     -0.017866   -0.950968   -1.427072
  O     -0.017865   -0.950968    1.427073
  O     -0.636251    1.672687    0.000000
  O      0.782883    1.623087   -0.000000

  5
IrO4+ minimum C d(O-O)=1.380
  Ir     0.012660   -0.089624    0.000001
  O     -0.018141   -0.957489   -1.424984
  O     -0.018140   -0.957489    1.424985
  O     -0.616147    1.679786    0.000000
  O      0.763292    1.631601    0.000000

  5
IrNO3 minimum A d(O-O)=2.830
  Ir      0.000000      0.000062     -0.012079
  O      -1.415036     -0.817069      0.530433
  O       1.415037     -0.817069      0.530434
  O       0.000000      1.634122      0.530470
  N      -0.000000     -0.000044     -1.686235

  5
IrNO3 d(O-O)=2.820
  O      -0.025000      0.014954      0.000544
  O       2.795000      0.014954      0.000544
  Ir      1.385000      1.001121     -0.000739
  N       1.385001      1.923909     -1.397588
  O       1.385001      2.064814      1.353223

  5
IrNO3 d(O-O)=2.770
  O      -0.025000      0.014682      0.000499
  O       2.745000      0.014682      0.000499
  Ir      1.360000      1.026851     -0.000688
  N       1.360001      1.945648     -1.400516
  O       1.360001      2.091244      1.352796

  5
IrNO3 d(O-O)=2.720
  O      -0.025000      0.014406      0.000456
  O       2.695000      0.014406      0.000456
  Ir      1.335000      1.052114     -0.000640
  N       1.335001      1.967120     -1.403314
  O       1.335001      2.117037      1.352530

  5
IrNO3 d(O-O)=2.670
  O      -0.025000      0.014105      0.000407
  O       2.645000      0.014106      0.000407
  Ir      1.310000      1.076864     -0.000585
  N       1.310001      1.988321     -1.405948
  O       1.310001      2.142164      1.352420

  5
IrNO3 d(O-O)=2.620
  O      -0.025000      0.013779      0.000351
  O       2.595000      0.013779      0.000351
  Ir      1.285000      1.101074     -0.000521
  N       1.285000      2.009223     -1.408415
  O       1.285000      2.166556      1.352489

  5
IrNO3 d(O-O)=2.570
  O      -0.025000      0.013526      0.000297
  O       2.545000      0.013526      0.000297
  Ir      1.260000      1.124786     -0.000461
  N       1.260000      2.029886     -1.410718
  O       1.260000      2.190277      1.352707

  5
IrNO3 d(O-O)=2.520
  O      -0.025000      0.013259      0.000237
  O       2.495000      0.013259      0.000237
  Ir      1.235000      1.147961     -0.000393
  N       1.235001      2.050397     -1.412773
  O       1.235001      2.213385      1.353016

  5
IrNO3 d(O-O)=2.470
  O      -0.025000      0.012947      0.000169
  O       2.445000      0.012947      0.000169
  Ir      1.210000      1.170550     -0.000314
  N       1.210000      2.070726     -1.414563
  O       1.210000      2.235801      1.353436

  5
IrNO3 d(O-O)=2.420
  O      -0.025000      0.012629      0.000104
  O       2.395000      0.012629      0.000104
  Ir      1.185000      1.192554     -0.000236
  N       1.185000      2.090818     -1.416126
  O       1.185000      2.257469      1.353985

  5
IrNO3 d(O-O)=2.370
  O      -0.025000      0.012361      0.000044
  O       2.345000      0.012361      0.000044
  Ir      1.160000      1.214029     -0.000163
  N       1.160000      2.110693     -1.417481
  O       1.160000      2.278451      1.354650

  5
IrNO3 d(O-O)=2.320
  O      -0.025000      0.012122     -0.000033
  O       2.295000      0.012122     -0.000032
  Ir      1.135000      1.234994     -0.000069
  N       1.135000      2.130472     -1.418537
  O       1.135000      2.298795      1.355437

  5
IrNO3 d(O-O)=2.270
  O      -0.025000      0.011853     -0.000125
  O       2.245000      0.011857     -0.000121
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  Ir      1.109997      1.255411      0.000044
  N       1.109998      2.150216     -1.419238
  O       1.109992      2.318452      1.356356

  5
IrNO3 d(O-O)=2.220
  O      -0.024979      0.011846     -0.000427
  O       2.195021      0.011736     -0.000164
  Ir      1.085083      1.275508      0.000228
  N       1.085294      2.170269     -1.419444
  O       1.084964      2.337412      1.357626

  5
IrNO3 d(O-O)=2.170
  O       0.027120      0.188410      0.017339
  O       2.195302      0.099998      0.008938
  Ir      1.163435      1.426259     -0.009842
  N       1.193714      2.295218     -1.445531
  O       1.212725      2.511052      1.328635

  5
IrNO3 TS B d(O-O)=2.122
  Ir      0.030205      0.185300     -0.124807
  O      -0.678910     -1.123648      0.781838
  O       1.426464     -0.968937      0.566433
  O       0.037885      1.801797      0.458323
  N       0.084356      0.105490     -1.788766

  5
IrNO3 d(O-O)=2.120
  O       0.007668      0.057340     -0.050680
  O       2.118275     -0.124194      0.031672
  Ir      1.401771      1.506958      0.017890
  N       1.448439      2.307852     -1.435807
  O       1.388446      2.540379      1.388936

  5
IrNO3 d(O-O)=2.070
  O       0.023758     -0.032306     -0.004045
  O       2.093678     -0.014040     -0.004702
  Ir      1.243985      1.583771      0.004779
  N       1.199625      2.354044     -1.462075
  O       1.231250      2.629467      1.365583

  5
IrNO3 d(O-O)=2.020
  O       0.028096     -0.014627     -0.002977
  O       2.048092     -0.018154     -0.001229
  Ir      1.214480      1.619265      0.002244
  N       1.203032      2.373311     -1.471402
  O       1.238575      2.671788      1.356877

  5
IrNO3 d(O-O)=1.970
  O       0.032988     -0.000068     -0.002952
  O       2.002817     -0.025939     -0.000953
  Ir      1.162130      1.648019      0.002085
  N       1.171230      2.389897     -1.475709
  O       1.210826      2.702267      1.353873

  5
IrNO3 d(O-O)=1.870
  O       0.024661     -0.007383      0.000046
  O       1.894660     -0.006074     -0.000407
  Ir      0.955529      1.687232      0.000415
  N       0.953957      2.417583     -1.481487
  O       0.953323      2.746110      1.348310

  5
IrNO3 d(O-O)=1.820
  O       0.024712     -0.007206     -0.000286
  O       1.844711     -0.005742     -0.000333
  Ir      0.932294      1.697480      0.000569
  N       0.931528      2.428015     -1.481130
  O       0.930423      2.758528      1.346544

  5
IrNO3 d(O-O)=1.770
  O       0.024907     -0.006526     -0.000371
  O       1.794907     -0.005960     -0.000246
  Ir      0.908972      1.707423      0.000539
  N       0.908854      2.437722     -1.481170
  O       0.908028      2.770720      1.344601

  5
IrNO3 d(O-O)=1.720
  O       0.024967     -0.006285     -0.000363
  O       1.744967     -0.006062     -0.000266
  Ir      0.884610      1.717118      0.000528
  N       0.884626      2.447146     -1.481186
  O       0.884169      2.782609      1.342752

  5
IrNO3 d(O-O)=1.670
  O       0.024990     -0.006134     -0.000350
  O       1.694990     -0.006049     -0.000294
  Ir      0.859858      1.726725      0.000515
  N       0.859890      2.456411     -1.481221
  O       0.859671      2.794372      1.340980

  5
IrNO3 d(O-O)=1.620
  O       0.024997     -0.006069     -0.000340
  O       1.644997     -0.006040     -0.000313
  Ir      0.834953      1.736233      0.000497
  N       0.834973      2.465555     -1.481256
  O       0.834882      2.806036      1.339275

  5
IrNO3 d(O-O)=1.570
  O       0.024999     -0.006107     -0.000336
  O       1.594999     -0.006099     -0.000325
  Ir      0.809985      1.745723      0.000480
  N       0.809994      2.474693     -1.481270
  O       0.809961      2.817709      1.337626

  5
IrNO3 d(O-O)=1.520
  O       0.025000     -0.006245     -0.000340
  O       1.545000     -0.006242     -0.000336
  Ir      0.784995      1.755331      0.000469
  N       0.784998      2.483971     -1.481258
  O       0.784988      2.829552      1.336026

  5
IrNO3 d(O-O)=1.470
  O       0.025000     -0.006478     -0.000350
  O       1.495000     -0.006478     -0.000348
  Ir      0.759999      1.765183      0.000467
  N       0.760000      2.493542     -1.481220
  O       0.759997      2.841747      1.334454

  5
IrNO3 d(O-O)=1.420
  O       0.025000     -0.006833     -0.000363
  O       1.445000     -0.006832     -0.000363
  Ir      0.734999      1.775435      0.000473
  N       0.735000      2.503575     -1.481179
  O       0.735000      2.854495      1.332900

  5
IrNO3 minimum C d(O-O)=1.408
  Ir     -0.016868      0.136255     -0.000008
  O      -1.312921      1.258976      0.004766
  O      -0.074391     -1.647697     -0.703926
  O      -0.069509     -1.647780      0.704174
  N       1.487281      0.816686     -0.005005

  5
IrNO3 minimum A d(N-O)=2.754
  Ir      0.000000      0.000062     -0.012079
  O      -1.415036     -0.817069      0.530433
  O       1.415037     -0.817069      0.530434
  O       0.000000      1.634122      0.530470
  N      -0.000000     -0.000044     -1.686235
```

```
  5
IrNO3 d(N-O)=2.750
  N      -0.025607      0.012980      0.000000
  O       2.724393      0.014270     -0.000000
  Ir      1.319586      1.008986     -0.000000
  O       1.270879      1.988433     -1.415259
  O       1.270879      1.988433      1.415259

  5
IrNO3 d(N-O)=2.700
  N      -0.025644      0.012727      0.000000
  O       2.674356      0.014098      0.000000
  Ir      1.294432      1.032834     -0.000000
  O       1.243110      2.010204     -1.416926
  O       1.243110      2.010204      1.416926

  5
IrNO3 d(N-O)=2.650
  N      -0.025694      0.012450     -0.000000
  O       2.624305      0.013944      0.000000
  Ir      1.269075      1.056354      0.000000
  O       1.215171      2.031597     -1.418631
  O       1.215171      2.031597      1.418631

  5
IrNO3 d(N-O)=2.600
  N      -0.025713      0.012252     -0.000000
  O       2.574287      0.013700     -0.000000
  Ir      1.243612      1.079531      0.000000
  O       1.187206      2.052612     -1.420362
  O       1.187206      2.052612      1.420362

  5
IrNO3 d(N-O)=2.550
  N      -0.025737      0.012099      0.000000
  O       2.524263      0.013501     -0.000000
  Ir      1.217932      1.102421     -0.000000
  O       1.159294      2.073285     -1.422129
  O       1.159294      2.073285      1.422129

  5
IrNO3 d(N-O)=2.500
  N      -0.025789      0.011928     -0.000000
  O       2.474211      0.013372     -0.000000
  Ir      1.191961      1.125008      0.000000
  O       1.131336      2.093704     -1.423872
  O       1.131336      2.093704      1.423872

  5
IrNO3 d(N-O)=2.450
  N      -0.025820      0.011830      0.000000
  O       2.424179      0.013169      0.000000
  Ir      1.165779      1.147300     -0.000000
  O       1.103448      2.113896     -1.425571
  O       1.103448      2.113896      1.425571

  5
IrNO3 d(N-O)=2.400
  N      -0.025860      0.011789     -0.000000
  O       2.374140      0.012952      0.000000
  Ir      1.139312      1.169351      0.000000
  O       1.075763      2.133870     -1.427253
  O       1.075763      2.133870      1.427253

  5
IrNO3 d(N-O)=2.350
  N      -0.025937      0.011816     -0.000000
  O       2.324063      0.012802      0.000000
  Ir      1.112405      1.191279     -0.000000
  O       1.048306      2.153690     -1.428949
  O       1.048306      2.153690      1.428949

  5
IrNO3 d(N-O)=2.300
  N      -0.026053      0.012050      0.000000
  O       2.273947      0.012766     -0.000000
  Ir      1.084923      1.213316     -0.000000
  O       1.021171      2.173555     -1.430679
  O       1.021171      2.173555      1.430679

  5
IrNO3 d(N-O)=2.250
  N      -0.026234      0.012564      0.000000
  O       2.223766      0.012844     -0.000000
  Ir      1.056643      1.235759     -0.000000
  O       0.994560      2.193782     -1.432430
  O       0.994560      2.193782      1.432430

  5
IrNO3 d(N-O)=2.200
  N      -0.026613      0.013633      0.000000
  O       2.173387      0.013372     -0.000000
  Ir      1.026982      1.259375     -0.000000
  O       0.968571      2.214947     -1.434298
  O       0.968571      2.214947      1.434298

  5
IrNO3 d(N-O)=2.150
  N      -0.053529      0.059037      0.000000
  O       2.095725      0.115687     -0.000000
  Ir      0.934168      1.356034     -0.000000
  O       0.857250      2.306691     -1.436661
  O       0.857250      2.306691      1.436661

  5
IrNO3 TS B' d(N-O)=2.103
  Ir      0.000000     -0.200540      0.074946
  O      -1.459676     -0.925170      0.605830
  O       1.459676     -0.925170      0.605830
  O      -0.000000      1.677747      0.128052
  N      -0.000000      0.373134     -1.521635

  5
IrNO3 d(N-O)=2.100
  N       0.028353     -0.016915      0.000000
  O       2.078244     -0.038020     -0.000000
  Ir      0.908846      1.484910      0.000000
  O       0.837711      2.357083     -1.467278
  O       0.837711      2.357083      1.467278

  5
IrNO3 d(N-O)=2.050
  N       0.024726     -0.014800      0.000000
  O       2.024724     -0.017692      0.000000
  Ir      0.877539      1.526369     -0.000000
  O       0.778872      2.390670     -1.467983
  O       0.778872      2.390670      1.467983

  5
IrNO3 d(N-O)=2.000
  N       0.023854     -0.014130      0.000000
  O       1.973853     -0.012051     -0.000000
  Ir      0.861091      1.553692     -0.000000
  O       0.746560      2.414003     -1.467372
  O       0.746560      2.414003      1.467372

  5
IrNO3 d(N-O)=1.950
  N       0.023818     -0.013266     -0.000000
  O       1.923816     -0.010216      0.000000
  Ir      0.848087      1.575712     -0.000000
  O       0.721889      2.434710     -1.465875
  O       0.721888      2.434710      1.465875

  5
IrNO3 d(N-O)=1.900
  N       0.024022     -0.012461     -0.000000
  O       1.874020     -0.009725      0.000000
  Ir      0.834954      1.594499      0.000000
  O       0.698911      2.454523     -1.463476
  O       0.698911      2.454523      1.463476

  5
IrNO3 d(N-O)=1.850
  N       0.024059     -0.011791     -0.000000
  O       1.824056     -0.008549      0.000000
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  Ir       0.820289      1.611762     -0.000000
  O        0.675989      2.473152     -1.461229
  O        0.675989      2.473152      1.461229

  5
IrNO3 d(N-O)=1.800
  N        0.024445     -0.010890      0.000000
  O        1.774444     -0.009032     -0.000000
  Ir       0.805318      1.627251      0.000000
  O        0.653879      2.491158     -1.458609
  O        0.653879      2.491158      1.458609

  5
IrNO3 d(N-O)=1.750
  N        0.024884     -0.009955      0.000000
  O        1.724884     -0.009918     -0.000000
  Ir       0.788106      1.641804     -0.000000
  O        0.629460      2.509068     -1.455635
  O        0.629460      2.509068      1.455635

5
IrNO3 d(N-O)=1.700
  N        0.025153     -0.009372     -0.000000
  O        1.675153     -0.010241      0.000000
  Ir       0.768026      1.655906      0.000000
  O        0.602094      2.526734     -1.452617
  O        0.602094      2.526734      1.452617

  5
IrNO3 d(N-O)=1.650
  N        0.025389     -0.009026      0.000000
  O        1.625388     -0.010674     -0.000000
  Ir       0.746168      1.669618     -0.000000
  O        0.573131      2.544286     -1.449536
  O        0.573131      2.544286      1.449536

  5
IrNO3 d(N-O)=1.600
  N        0.025686     -0.008728     -0.000000
  O        1.575683     -0.011658      0.000000
  Ir       0.722858      1.683183     -0.000000
  O        0.542523      2.562170     -1.446256
  O        0.542522      2.562170      1.446256

  5
IrNO3 d(N-O)=1.550
  N        0.025952     -0.008667      0.000000
  O        1.525947     -0.012699     -0.000000
  Ir       0.697478      1.697042      0.000000
  O        0.509274      2.580645     -1.442845
  O        0.509274      2.580645      1.442845

  5
IrNO3 d(N-O)=1.500
  N        0.026224     -0.009125      0.000000
  O        1.476216     -0.014065      0.000000
  Ir       0.670219      1.711298     -0.000000
  O        0.473501      2.600301     -1.438945
  O        0.473501      2.600301      1.438945

  5
IrNO3 d(N-O)=1.450
  N        0.026417     -0.008628     -0.000000
  O        1.426402     -0.014928      0.000000
  Ir       0.641400      1.727112     -0.000000
  O        0.435339      2.620461     -1.435894
  O        0.435339      2.620461      1.435894

  5
IrNO3 d(N-O)=1.400
  N        0.026867     -0.009113      0.000000
  O        1.376839     -0.017858     -0.000000
  Ir       0.610933      1.743055      0.000000
  O        0.393350      2.642106     -1.431813
  O        0.393350      2.642106      1.431813

  5
IrNO3 d(N-O)=1.350
  N        0.027172     -0.008946     -0.000000
  O        1.327126     -0.019902      0.000000
  Ir       0.577008      1.761458      0.000000
  O        0.345000      2.665191     -1.428273
  O        0.345000      2.665191      1.428273

  5
IrNO3 minimum C' d(N-O)=1.315
  Ir      -0.073922     -0.075331      0.000000
  O        0.027842     -1.000178     -1.429487
  O        0.027840     -1.000178      1.429488
  O       -0.579796      1.785590      0.000003
  N        0.721562      1.596882     -0.000000

  5
IrN2O2- minimum A d(O-O)=2.900
  Ir      -0.730041      0.260616     -0.161472
  O       -0.135230      1.077960      1.289655
  O       -0.160676      1.092504     -1.614535
  N       -0.166695     -1.348937     -0.174455
  N       -2.435322      0.252469     -0.146650

  5
IrN2O2- d(O-O)=2.846
  Ir      -0.600375      0.153082      0.014026
  O       -2.361964      0.151148     -0.010560
  O       -0.043265      0.986120     -1.434856
  N       -0.015707     -1.449218      0.026207
  N       -0.037531      0.963782      1.405184

  5
IrN2O2- d(O-O)=2.793
  Ir      -0.593990      0.148690      0.021839
  O       -2.349043      0.165155     -0.034853
  O       -0.073993      0.984385     -1.432373
  N       -0.009978     -1.454176      0.032597
  N       -0.031837      0.960860      1.412791

  5
IrN2O2- d(O-O)=2.730
  Ir      -0.587683      0.144346      0.029506
  O       -2.335957      0.179106     -0.058939
  O       -0.104589      0.982580     -1.429746
  N       -0.004321     -1.459087      0.038906
  N       -0.026292      0.957970      1.420274

  5
IrN2O2- d(O-O)=2.686
  Ir      -0.581489      0.140081      0.037033
  O       -2.322737      0.192946     -0.082867
  O       -0.135047      0.980692     -1.426938
  N        0.001240     -1.463908      0.045145
  N       -0.020809      0.955104      1.427626

  5
IrN2O2- d(O-O)=2.632
  Ir      -0.575427      0.135928      0.044407
  O       -2.309346      0.206593     -0.106628
  O       -0.165335      0.978722     -1.423901
  N        0.006631     -1.468620      0.051297
  N       -0.015365      0.952290      1.434826

  5
IrN2O2- d(O-O)=2.579
  Ir      -0.569504      0.131854      0.051636
  O       -2.295808      0.220097     -0.130213
  O       -0.195450      0.976660     -1.420616
  N        0.011901     -1.473233      0.057348
  N       -0.009980      0.949536      1.441845

  5
IrN2O2- d(O-O)=2.525
  Ir      -0.563755      0.127855      0.058717
  O       -2.282131      0.233524     -0.153569
  O       -0.225360      0.974409     -1.417058
  N        0.017120     -1.477713      0.063228
  N       -0.004715      0.946839      1.448682
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  5
IrN2O2- d(O-O)=2.471
  Ir    -0.558170    0.123948    0.065621
  O     -2.268296    0.246896   -0.176682
  O     -0.255088    0.971975   -1.413297
  N      0.022304   -1.482044    0.068985
  N      0.000408    0.944139    1.455374

  5
IrN2O2- d(O-O)=2.418
  Ir    -0.552697    0.120160    0.072313
  O     -2.254227    0.260143   -0.199546
  O     -0.284661    0.969448   -1.409392
  N      0.027359   -1.486246    0.074690
  N      0.005385    0.941408    1.461937

  5
IrN2O2- d(O-O)=2.364
  Ir    -0.547379    0.116499    0.078826
  O     -2.239980    0.273234   -0.222209
  O     -0.314054    0.966791   -1.405271
  N      0.032285   -1.490288    0.080306
  N      0.010285    0.938677    1.468349

  5
IrN2O2- d(O-O)=2.311
  Ir    -0.542220    0.112960    0.085156
  O     -2.225567    0.286164   -0.244692
  O     -0.343275    0.964032   -1.400924
  N      0.037084   -1.494172    0.085863
  N      0.015137    0.935930    1.474598

  5
IrN2O2- d(O-O)=2.257
  Ir    -0.537190    0.109535    0.091278
  O     -2.210956    0.298965   -0.266955
  O     -0.372345    0.961188   -1.396410
  N      0.041769   -1.497914    0.091391
  N      0.019880    0.933139    1.480697

  5
IrN2O2- d(O-O)=2.204
  Ir    -0.532340    0.106191    0.097197
  O     -2.196207    0.311699   -0.289015
  O     -0.401245    0.958227   -1.391665
  N      0.046419   -1.501485    0.096893
  N      0.024531    0.930281    1.486590

  5
IrN2O2- TS B d(O-O)=2.150
  Ir    -0.586303    0.018669    0.249472
  O     -2.207634    0.373566   -0.397762
  O     -0.466516    1.014163   -1.490144
  N      0.111750   -1.527722    0.118177
  N      0.089861    0.926238    1.520258

  5
IrN2O2- d(O-O)=2.096
  Ir    -0.553156    0.012217    0.261246
  O     -2.186887    0.390393   -0.426937
  O     -0.519979    1.033055   -1.523940
  N      0.111557   -1.547646    0.140789
  N      0.089624    0.916894    1.548844

  5
IrN2O2- d(O-O)=2.043
  Ir    -0.526203    0.011552    0.262826
  O     -2.170780    0.404530   -0.451010
  O     -0.561967    1.040278   -1.537662
  N      0.111144   -1.559750    0.157785
  N      0.088964    0.908304    1.568062

  5
IrN2O2- d(O-O)=1.898
  Ir    -0.498926    0.012681    0.261395
  O     -2.157955    0.418539   -0.475061
  O     -0.600762    1.043174   -1.543817
  N      0.110555   -1.569712    0.172897
  N      0.088246    0.900232    1.584588

  5
IrN2O2- d(O-O)=1.936
  Ir    -0.471046    0.015144    0.257638
  O     -2.151322    0.433360   -0.500915
  O     -0.635470    1.040734   -1.540280
  N      0.110638   -1.577640    0.185550
  N      0.088358    0.893315    1.598008

  5
IrN2O2- d(O-O)=1.882
  Ir    -0.441265    0.019530    0.250376
  O     -2.158460    0.451151   -0.532713
  O     -0.663398    1.028892   -1.519358
  N      0.113148   -1.582873    0.194749
  N      0.091135    0.888213    1.606947

  5
IrN2O2- d(O-O)=1.829
  Ir    -0.417773    0.024355    0.242080
  O     -2.181920    0.474223   -0.573852
  O     -0.680695    1.003217   -1.473942
  N      0.121707   -1.583275    0.197433
  N      0.099839    0.886394    1.608283

  5
IrN2O2- d(O-O)=1.875
  Ir    -0.415725    0.022715    0.244996
  O     -2.163420    0.484503   -0.591451
  O     -0.706200    0.997945   -1.465244
  N      0.124197   -1.584484    0.200670
  N      0.102306    0.884234    1.611030

  5
IrN2O2- d(O-O)=1.721
  Ir    -0.413656    0.021187    0.247722
  O     -2.144712    0.494656   -0.608810
  O     -0.731640    0.992631   -1.456491
  N      0.126545   -1.585915    0.203706
  N      0.104621    0.882354    1.613874

  5
IrN2O2- d(O-O)=1.668
  Ir    -0.411580    0.019700    0.250377
  O     -2.125847    0.504721   -0.625947
  O     -0.756933    0.987180   -1.447565
  N      0.128754   -1.587324    0.206526
  N      0.106764    0.880636    1.616610

  5
IrN2O2- d(O-O)=1.614
  Ir    -0.409475    0.018231    0.252999
  O     -2.106906    0.514739   -0.642959
  O     -0.782130    0.981634   -1.438506
  N      0.130873   -1.588835    0.209136
  N      0.108796    0.879145    1.619332

  5
IrN2O2- d(O-O)=1.561
  Ir    -0.407228    0.016695    0.255753
  O     -2.087711    0.524639   -0.659633
  O     -0.807124    0.975889   -1.429242
  N      0.132724   -1.590516    0.211169
  N      0.110497    0.878207    1.621954

  5
IrN2O2- d(O-O)=1.507
  Ir    -0.405045    0.015186    0.258443
  O     -2.068768    0.534609   -0.676621
  O     -0.832228    0.970285   -1.420015
  N      0.134749   -1.592200    0.213521
  N      0.112451    0.877034    1.624673

  5
IrN2O2- d(O-O)=1.454
  Ir    -0.402779    0.013612    0.261238
  O     -2.049927    0.544528   -0.693792
```

```
  O     -0.857401    0.964846   -1.410788
  N      0.136763   -1.594037    0.215890
  N      0.114502    0.875966    1.627452

  5
Structure minimum C d(O-O)=1.440
  Ir     0.000099   -0.001917   -0.184526
  O      0.677604    0.005547    1.671996
  O     -0.759580    0.009510    1.640154
  N      0.016853   -1.429421   -1.101089
  N      0.024985    1.416022   -1.115643

  5
IrN2O2- minimum A d(N-O)=2.840
  Ir    -0.730041    0.260616   -0.161472
  O     -0.135230    1.077960    1.289655
  O     -0.160676    1.092504   -1.614535
  N     -0.166695   -1.348937   -0.174455
  N     -2.435322    0.252469   -0.146650

  5
IrN2O2- d(N-O)=2.796
  Ir    -0.725070    0.257758   -0.156473
  O     -0.158708    0.971668    1.359291
  O     -0.118699    1.163606   -1.542520
  N     -0.200841   -1.362647   -0.252848
  N     -2.424647    0.304230   -0.214908

  5
IrN2O2- d(N-O)=2.742
  Ir    -0.718048    0.253614   -0.148716
  O     -0.153828    0.968710    1.367516
  O     -0.149107    1.161924   -1.540685
  N     -0.196756   -1.368215   -0.247334
  N     -2.410225    0.318580   -0.238238

  5
IrN2O2- d(N-O)=2.688
  Ir    -0.711218    0.249454   -0.140966
  O     -0.148967    0.965866    1.375625
  O     -0.179375    1.160176   -1.538703
  N     -0.192728   -1.373720   -0.241951
  N     -2.395677    0.332839   -0.261462

  5
IrN2O2- d(N-O)=2.635
  Ir    -0.704549    0.245320   -0.133254
  O     -0.144159    0.963042    1.383683
  O     -0.209535    1.158406   -1.536705
  N     -0.188791   -1.379146   -0.236614
  N     -2.380930    0.346991   -0.284567

  5
IrN2O2- d(N-O)=2.581
  Ir    -0.698071    0.241199   -0.125589
  O     -0.139419    0.960259    1.391650
  O     -0.239566    1.156603   -1.534647
  N     -0.184929   -1.384494   -0.231345
  N     -2.365980    0.361047   -0.307525

  5
IrN2O2- d(N-O)=2.527
  Ir    -0.691845    0.237029   -0.117930
  O     -0.134726    0.957535    1.399475
  O     -0.269457    1.154775   -1.532495
  N     -0.181080   -1.389779   -0.226155
  N     -2.350857    0.375054   -0.330352

  5
IrN2O2- d(N-O)=2.473
  Ir    -0.685948    0.232798   -0.110201
  O     -0.129982    0.954904    1.407149
  O     -0.299185    1.152880   -1.530195
  N     -0.177227   -1.394958   -0.221090
  N     -2.335623    0.388991   -0.353120

  5
IrN2O2- d(N-O)=2.419
  Ir    -0.680458    0.228463   -0.102297
  O     -0.125095    0.952426    1.414657
  O     -0.328727    1.150932   -1.527712
  N     -0.173388   -1.400021   -0.216193
  N     -2.320298    0.402814   -0.375912

  5
IrN2O2- d(N-O)=2.365
  Ir    -0.675425    0.223960   -0.094122
  O     -0.120021    0.950054    1.422040
  O     -0.358126    1.149032   -1.525183
  N     -0.169531   -1.404993   -0.211397
  N     -2.304862    0.416560   -0.398795

  5
IrN2O2- d(N-O)=2.312
  Ir    -0.670967    0.219177   -0.085487
  O     -0.114668    0.947707    1.429365
  O     -0.387445    1.147250   -1.522796
  N     -0.165521   -1.409866   -0.206636
  N     -2.289364    0.430346   -0.421903

  5
IrN2O2- d(N-O)=2.258
  Ir    -0.667317    0.213902   -0.075913
  O     -0.108843    0.945345    1.436802
  O     -0.416752    1.145588   -1.520872
  N     -0.161146   -1.414574   -0.201972
  N     -2.273906    0.444353   -0.445502
  5
IrN2O2- d(N-O)=2.204
  Ir    -0.664714    0.207373   -0.064321
  O     -0.102355    0.943130    1.444687
  O     -0.446311    1.144455   -1.520265
  N     -0.156032   -1.419410   -0.197512
  N     -2.258553    0.459066   -0.470047

  5
IrN2O2- TS B' d(N-O)=2.150
  Ir    -0.646128    0.158454    0.025890
  O     -0.080990    0.933133    1.502338
  O     -0.517064    1.186629   -1.615319
  N     -0.137869   -1.445666   -0.180568
  N     -2.245914    0.502064   -0.539798

  5
IrN2O2- d(N-O)=2.097
  Ir    -0.614066    0.151285    0.042115
  O     -0.083253    0.922114    1.529678
  O     -0.562346    1.193903   -1.644285
  N     -0.136864   -1.456183   -0.168037
  N     -2.231437    0.523495   -0.566928

  5
IrN2O2- d(N-O)=2.043
  Ir    -0.594028    0.149069    0.047245
  O     -0.083748    0.914821    1.543079
  O     -0.596293    1.191060   -1.647984
  N     -0.134757   -1.461324   -0.159638
  N     -2.219138    0.540989   -0.590159

  5
IrN2O2- d(N-O)=1.990
  Ir    -0.577622    0.147961    0.049784
  O     -0.083555    0.908797    1.552533
  O     -0.626694    1.185575   -1.644731
  N     -0.132410   -1.464918   -0.152644
  N     -2.207685    0.557198   -0.612399

  5
IrN2O2- d(N-O)=1.937
  Ir    -0.563779    0.147458    0.051173
  O     -0.082840    0.903056    1.560078
  O     -0.655365    1.179058   -1.638540
  N     -0.129824   -1.467612   -0.146075
  N     -2.196157    0.572654   -0.634093

  5
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IrN2O2- d(N-O)=1.883

Ir	-0.551944	0.147144	0.052025
O	-0.081784	0.897636	1.566429
O	-0.683055	1.172493	-1.630938
N	-0.127267	-1.469953	-0.139689
N	-2.183916	0.587294	-0.655284

5

IrN2O2- d(N-O)=1.830

Ir	-0.541784	0.147138	0.052625
O	-0.080333	0.892180	1.572172
O	-0.710147	1.165838	-1.622739
N	-0.124698	-1.471827	-0.133393
N	-2.171004	0.601286	-0.676123

5

IrN2O2- d(N-O)=1.777

Ir	-0.532836	0.146792	0.053235
O	-0.078992	0.887488	1.577215
O	-0.736699	1.159360	-1.613965
N	-0.122193	-1.473859	-0.127627
N	-2.157245	0.614832	-0.696314

5

IrN2O2- d(N-O)=1.723

Ir	-0.524781	0.146442	0.053833
O	-0.077882	0.882726	1.582248
O	-0.763439	1.153552	-1.606197
N	-0.119915	-1.475901	-0.121747
N	-2.141947	0.627795	-0.715595

5

IrN2O2- d(N-O)=1.670

Ir	-0.517471	0.146061	0.054509
O	-0.076658	0.877877	1.587290
O	-0.790306	1.148309	-1.599011
N	-0.117710	-1.477965	-0.115679
N	-2.125819	0.640332	-0.734566

5

IrN2O2- d(N-O)=1.617

Ir	-0.510828	0.145610	0.055303
O	-0.075269	0.872950	1.592371
O	-0.817239	1.143373	-1.592237
N	-0.115423	-1.480009	-0.109503
N	-2.109206	0.652690	-0.753390

5

IrN2O2- d(N-O)=1.563

Ir	-0.504664	0.145087	0.056226
O	-0.073666	0.867810	1.597638
O	-0.844443	1.138961	-1.586132
N	-0.113061	-1.482107	-0.103009
N	-2.092131	0.664863	-0.772180

5

IrN2O2- d(N-O)=1.510

Ir	-0.498673	0.144641	0.057106
O	-0.071803	0.861991	1.603465
O	-0.872339	1.135303	-1.581300
N	-0.110473	-1.484373	-0.095674
N	-2.074677	0.677053	-0.791054

5

IrN2O2- d(N-O)=1.457

Ir	-0.492684	0.144028	0.058227
O	-0.069879	0.856084	1.609649
O	-0.900697	1.132166	-1.577320
N	-0.107841	-1.486874	-0.088119
N	-2.056865	0.689210	-0.809894

5

IrN2O2- d(N-O)=1.403

Ir	-0.486393	0.143379	0.059458
O	-0.067823	0.849664	1.616545
O	-0.929914	1.129736	-1.574733
N	-0.105018	-1.489711	-0.079873
N	-2.038816	0.701547	-0.828853

5

IrN2O2- minimum C' d(N-O)=1.370

Ir	0.014816	0.127446	0.073596
O	-1.337717	1.249591	-0.047931
O	-0.068286	-1.740407	0.680743
N	1.523036	0.867938	-0.031086
N	-0.118256	-1.588128	-0.675320

5

IrN2O2- minimum A d(N-N)=2.780

Ir	-0.730041	0.260616	-0.161472
O	-0.135230	1.077960	1.289655
O	-0.160676	1.092504	-1.614535
N	-0.166695	-1.348937	-0.174455
N	-2.435322	0.252469	-0.146650

5

IrN2O2- d(N-N)=2.734

Ir	-0.605623	0.156770	0.007466
O	-0.006693	-1.508592	-0.001746
O	-0.029592	1.017987	1.442296
N	-2.296547	0.174436	-0.050052
N	-0.120386	0.964313	-1.397962

5

IrN2O2- d(N-N)=2.679

Ir	-0.599642	0.152670	0.014666
O	-0.001466	-1.513735	0.003769
O	-0.024404	1.015926	1.449486
N	-2.282161	0.188249	-0.073967
N	-0.151168	0.961803	-1.393953

5

IrN2O2- d(N-N)=2.623

Ir	-0.593733	0.148648	0.021779
O	0.003680	-1.518783	0.009228
O	-0.019267	1.013865	1.456610
N	-2.267668	0.201973	-0.097772
N	-0.181854	0.959212	-1.389844

5

IrN2O2- d(N-N)=2.568

Ir	-0.587919	0.144691	0.028818
O	0.008748	-1.523728	0.014577
O	-0.014180	1.011846	1.463629
N	-2.253079	0.215600	-0.121451
N	-0.212411	0.956505	-1.385570

5

IrN2O2- d(N-N)=2.512

Ir	-0.582211	0.140778	0.035784
O	0.013749	-1.528576	0.019772
O	-0.009178	1.009901	1.470502
N	-2.238389	0.229152	-0.144973
N	-0.242811	0.953659	-1.381084

5

IrN2O2- d(N-N)=2.457

Ir	-0.576572	0.136868	0.042675
O	0.018607	-1.533391	0.024755
O	-0.004344	1.008128	1.477156
N	-2.223517	0.242593	-0.168257
N	-0.273014	0.950716	-1.376327

5

IrN2O2- d(N-N)=2.401

Ir	-0.571064	0.133043	0.049393
O	0.023495	-1.538045	0.029951
O	0.000556	1.006108	1.483733
N	-2.208621	0.256002	-0.191531
N	-0.303206	0.947806	-1.371544

5

IrN2O2- d(N-N)=2.346

Ir	-0.565634	0.129323	0.055997
O	0.028317	-1.542505	0.035172
O	0.005426	1.003959	1.490241

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  N     -2.193626    0.269327   -0.214705
  N     -0.333324    0.944809   -1.366702

  5
IrN2O2- TS B" DFT(B3LYP)/ZORA d(N-N)=2.290
  Ir    -0.606392    0.052900    0.189220
  O      0.086973   -1.565992    0.075269
  O      0.063964    0.982108    1.531511
  N     -2.192382    0.334300   -0.328338
  N     -0.411005    1.001599   -1.467661

  5
IrN2O2- d(N-N)=2.238
  Ir    -0.413434    0.025252    0.240685
  O      0.172773   -1.627544    0.218462
  O      0.150076    0.891068    1.657981
  N     -1.987781    0.575330   -0.746570
  N     -0.980474    0.940808   -1.370556

  5
IrN2O2- d(N-N)=1.185
  Ir    -0.418305    0.028423    0.235001
  O      0.163603   -1.623504    0.206016
  O      0.140920    0.899664    1.647992
  N     -1.997533    0.559583   -0.719406
  N     -0.947525    0.940748   -1.369601

  5
IrN2O2- d(N-N)=2.133
  Ir    -0.422238    0.031210    0.230009
  O      0.155357   -1.620257    0.194624
  O      0.132518    0.907703    1.639340
  N     -2.008542    0.544882   -0.693596
  N     -0.915936    0.941376   -1.370375

  5
IrN2O2- d(N-N)=2.090
  Ir    -0.425678    0.033561    0.225802
  O      0.147768   -1.617750    0.183905
  O      0.124900    0.915590    1.631606
  N     -2.020549    0.530716   -0.669100
  N     -0.885282    0.942798   -1.372211

  5
IrN2O2- d(N-N)=2.040
  Ir    -0.428436    0.035692    0.222007
  O      0.140713   -1.615789    0.173843
  O      0.117730    0.923155    1.624757
  N     -2.033329    0.517165   -0.645445
  N     -0.855520    0.944692   -1.375161

  5
IrN2O2- d(N-N)=1.990
  Ir    -0.431218    0.037385    0.218994
  O      0.134243   -1.614266    0.164127
  O      0.111235    0.930681    1.618426
  N     -2.046835    0.504051   -0.622799
  N     -0.826265    0.947063   -1.378746

  5
IrN2O2- d(N-N)=1.940
  Ir    -0.433589    0.038969    0.216170
  O      0.128212   -1.613054    0.155087
  O      0.105141    0.937777    1.612720
  N     -2.060906    0.491356   -0.600804
  N     -0.797699    0.949867   -1.383172

  5
IrN2O2- d(N-N)=1.890
  Ir    -0.435742    0.040444    0.213549
  O      0.122557   -1.612044    0.146577
  O      0.099436    0.944524    1.607465
  N     -2.075462    0.478979   -0.579396
  N     -0.769630    0.953011   -1.388194

  5
IrN2O2- d(N-N)=1.840
  Ir    -0.437821    0.041837    0.211085
  O      0.117282   -1.611120    0.138570
  O      0.094139    0.950890    1.602550
  N     -2.090497    0.466897   -0.558554
  N     -0.741944    0.956410   -1.393649

  5
IrN2O2- d(N-N)=1.790
  Ir    -0.439836    0.043189    0.208706
  O      0.112291   -1.610232    0.130942
  O      0.089089    0.956933    1.597903
  N     -2.105829    0.455061   -0.538052
  N     -0.714556    0.959963   -1.399498

  5
IrN2O2- d(N-N)=1.740
  Ir    -0.441801    0.044537    0.206335
  O      0.107491   -1.609357    0.123711
  O      0.084269    0.962656    1.593451
  N     -2.121369    0.443341   -0.517833
  N     -0.687432    0.963737   -1.405661

  5
IrN2O2- d(N-N)=1.690
  Ir    -0.443576    0.045782    0.204145
  O      0.102570   -1.608767    0.116124
  O      0.079270    0.968810    1.589096
  N     -2.136808    0.431618   -0.497495
  N     -0.660296    0.967472   -1.411868

  5
IrN2O2- d(N-N)=1.640
  Ir    -0.525416    0.100628    0.106978
  O      0.065284   -1.574887    0.075197
  O      0.042560    0.986483    1.538763
  N     -2.080276    0.370416   -0.390326
  N     -0.560993    0.922273   -1.330610

  5
IrN2O2- d(N-N)=1.590
  Ir    -0.530076    0.104997    0.099190
  O      0.060038   -1.570009    0.070409
  O      0.037192    0.988030    1.532066
  N     -2.093871    0.357292   -0.367327
  N     -0.532124    0.924604   -1.334337

  5
IrN2O2- d(N-N)=1.540
  Ir    -0.535641    0.108856    0.092361
  O      0.055698   -1.565811    0.065734
  O      0.032730    0.989813    1.526147
  N     -2.107995    0.344740   -0.345317
  N     -0.503633    0.927316   -1.338923

  5
IrN2O2- d(N-N)=1.490
  Ir    -0.540761    0.112421    0.086121
  O      0.051151   -1.561913    0.060596
  O      0.028151    0.992160    1.520287
  N     -2.122183    0.332163   -0.323430
  N     -0.475199    0.930084   -1.343573

  5
IrN2O2- d(N-N)=1.440
  Ir    -0.545743    0.115851    0.080094
  O      0.046584   -1.558115    0.055432
  O      0.023624    0.994612    1.514422
  N     -2.136470    0.319591   -0.301691
  N     -0.446836    0.932976   -1.348254

  5
IrN2O2- d(N-N)=1.390
  Ir    -0.550677    0.119203    0.074143
  O      0.042020   -1.554334    0.050267
  O      0.019081    0.997085    1.508494
  N     -2.150783    0.307042   -0.279978
  N     -0.418483    0.935917   -1.352923

  5
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```
IrN2O2- d(N-N)=1.340
  Ir    -0.555608    0.122549    0.068173
  O      0.037449   -1.550496    0.045148
  O      0.014523    0.999496    1.502500
  N     -2.165082    0.294489   -0.258248
  N     -0.390123    0.938875   -1.357572

  5
IrN2O2- d(N-N)=1.290
  Ir    -0.560596    0.125918    0.062125
  O      0.032892   -1.546557    0.040147
  O      0.009998    1.001772    1.496418
  N     -2.179384    0.281919   -0.236519
  N     -0.361751    0.941863   -1.362168

  5
IrN2O2- minimum C" d(N-N)=1.240
  Ir     0.015687   -0.078602   -0.000000
  O     -0.010202   -1.064592   -1.450265
  O     -0.010194   -1.064591    1.450266
  N     -0.555372    1.773723   -0.000008
  N      0.683608    1.740846    0.000008

  5
PtO4_2+ minimum A d(O-O)= 2.790
  O      0.000639    0.001557    0.000000
  O      2.790638    0.000310   -0.000000
  Pt     1.396064    0.985945    0.000000
  O      1.396479    1.971586   -1.394324
  O      1.396479    1.971586    1.394324

  5
PtO4_2+ d(O-O)= 2.740
  O      0.024989   -0.014746   -0.000000
  O      2.764989   -0.014711    0.000000
  Pt     1.394982    0.995961    0.000000
  O      1.394973    1.979907   -1.394995
  O      1.394973    1.979907    1.394995

  5
PtO4_2+ d(O-O)= 2.690
  O      0.025002   -0.014569   -0.000000
  O      2.715002   -0.014573    0.000000
  Pt     1.370004    1.021403   -0.000000
  O      1.370008    2.003849   -1.395591
  O      1.370008    2.003849    1.395591

  5
PtO4_2+ d(O-O)= 2.640
  O      0.025001   -0.014345    0.000000
  O      2.665001   -0.014347    0.000000
  Pt     1.345002    1.046429    0.000000
  O      1.345002    2.027539   -1.396167
  O      1.345002    2.027538    1.396167

  5
PtO4_2+ d(O-O)= 2.590
  O      0.025000   -0.014039   -0.000000
  O      2.615000   -0.014039   -0.000000
  Pt     1.320000    1.070985   -0.000000
  O      1.319999    2.050819   -1.396755
  O      1.319999    2.050819    1.396755

  5
PtO4_2+ d(O-O)= 2.540
  O      0.025000   -0.013746    0.000000
  O      2.565000   -0.013746    0.000000
  Pt     1.295001    1.094971    0.000000
  O      1.294999    2.073631   -1.397328
  O      1.294999    2.073630    1.397328

  5
PtO4_2+ d(O-O)= 2.490
  O      0.025000   -0.013659   -0.000000
  O      2.515000   -0.013660   -0.000000
  Pt     1.270001    1.118264   -0.000000
  O      1.269999    2.096262   -1.397471
  O      1.269999    2.096262    1.397471

  5
PtO4_2+ d(O-O)= 2.440
  O      0.025000   -0.013394   -0.000000
  O      2.465000   -0.013394   -0.000000
  Pt     1.245000    1.141225   -0.000000
  O      1.244999    2.118665   -1.397761
  O      1.244999    2.118665    1.397761

  5
PtO4_2+ d(O-O)= 2.390
  O      0.025000   -0.013138   -0.000000
  O      2.415000   -0.013138   -0.000000
  Pt     1.220000    1.163653    0.000000
  O      1.220000    2.140680   -1.397984
  O      1.220000    2.140680    1.397984

  5
PtO4_2+ d(O-O)= 2.340
  O      0.025000   -0.012883   -0.000000
  O      2.365000   -0.012884   -0.000000
  Pt     1.195000    1.185564    0.000000
  O      1.195000    2.162314   -1.398152
  O      1.195000    2.162314    1.398152

  5
PtO4_2+ d(O-O)= 2.290
  O      0.025000   -0.012663    0.000000
  O      2.315000   -0.012664    0.000000
  Pt     1.170000    1.206944    0.000000
  O      1.170000    2.183614   -1.398219
  O      1.170000    2.183614    1.398219

  5
PtO4_2+ d(O-O)= 2.240
  O      0.025000   -0.012532   -0.000000
  O      2.265000   -0.012533   -0.000000
  Pt     1.145000    1.227811   -0.000000
  O      1.144999    2.204708   -1.398123
  O      1.145000    2.204708    1.398123

  5
PtO4_2+ d(O-O)= 2.190
  O      0.025000   -0.012403    0.000000
  O      2.215000   -0.012403    0.000000
  Pt     1.120000    1.248280    0.000000
  O      1.120000    2.225675   -1.397885
  O      1.120000    2.225675    1.397885

  5
PtO4_2+ d(O-O)= 2.140
  O      0.025000   -0.012296    0.000000
  O      2.165000   -0.012296   -0.000000
  Pt     1.095000    1.268376    0.000000
  O      1.095000    2.246527   -1.397516
  O      1.095000    2.246527    1.397516

  5
PtO4_2+ d(O-O)= 2.090
  O      0.025000   -0.012248   -0.000000
  O      2.115000   -0.012248    0.000000
  Pt     1.070000    1.288147   -0.000000
  O      1.070000    2.267334   -1.397015
  O      1.070000    2.267334    1.397015

  5
PtO4_2+ d(O-O)= 2.040
  O      0.025000   -0.012253    0.000000
  O      2.065000   -0.012254   -0.000000
  Pt     1.045001    1.307704    0.000000
  O      1.045000    2.288180   -1.396420
  O      1.045000    2.288180    1.396420

  5
PtO4_2+ d(O-O)= 1.990
  O      0.025000   -0.012277   -0.000000
  O      2.015000   -0.012276   -0.000000
  Pt     1.019999    1.327200   -0.000000
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  O      1.019999    2.309089   -1.395847
  O      1.019999    2.309089    1.395847

  5
PtO4_2+ d(O-O)= 1.940
  O      0.025000   -0.012381    0.000000
  O      1.965000   -0.012381    0.000000
  Pt     0.995000    1.346765    0.000000
  O      0.995000    2.330102   -1.395394
  O      0.995000    2.330102    1.395394

  5
PtO4_2+ d(O-O)= 1.890
  O      0.025013   -0.012636    0.000000
  O      1.915013   -0.012747    0.000000
  Pt     0.970046    1.366671    0.000000
  O      0.969964    2.351413   -1.395193
  O      0.969964    2.351412    1.395192

  5
PtO4_2+ d(O-O)= 1.840
  O      0.024995   -0.113703   -0.000000
  O      1.864995   -0.113596   -0.000000
  Pt     0.944896    1.546258   -0.000000
  O      0.944845    2.394306   -1.456290
  O      0.944845    2.394306    1.456290

  5
PtO4_2+ d(O-O)= 1.790
  O      0.025000   -0.008318    0.000000
  O      1.815000   -0.008316   -0.000000
  Pt     0.919998    1.663658   -0.000000
  O      0.919997    2.514398   -1.454202
  O      0.919997    2.514397    1.454202

  5
PtO4_2+ d(O-O)= 1.740
  O      0.025000   -0.009942    0.000000
  O      1.765000   -0.009944   -0.000000
  Pt     0.895002    1.674695    0.000000
  O      0.894999    2.531298   -1.450541
  O      0.894999    2.531297    1.450541

  5
PtO4_2+ d(O-O)= 1.690
  O      0.025000   -0.009976   -0.000000
  O      1.715000   -0.009976    0.000000
  Pt     0.870002    1.687660    0.000000
  O      0.869996    2.549706   -1.447118
  O      0.869996    2.549706    1.447118

  5
PtO4_2+ d(O-O)= 1.640
  O      0.025000   -0.010376   -0.000000
  O      1.665000   -0.010376   -0.000000
  Pt     0.845000    1.700731   -0.000000
  O      0.844995    2.568510   -1.443546
  O      0.844995    2.568510    1.443546

  5
PtO4_2+ d(O-O)= 1.590
  O      0.025000   -0.010979    0.000000
  O      1.615000   -0.010978    0.000000
  Pt     0.820000    1.714298    0.000000
  O      0.819996    2.588270   -1.439750
  O      0.819996    2.588270    1.439750

  5
PtO4_2+ d(O-O)= 1.540
  O      0.025000   -0.011776   -0.000000
  O      1.565000   -0.011777    0.000000
  Pt     0.795002    1.728667   -0.000000
  O      0.794996    2.609330   -1.435719
  O      0.794996    2.609330    1.435719

  5
PtO4_2+ d(O-O)= 1.490
  O      0.024999   -0.012852    0.000000
  O      1.514999   -0.012862    0.000000
  Pt     0.770015    1.744133    0.000000
  O      0.769987    2.632118   -1.431367
  O      0.769987    2.632117    1.431367

  5
PtO4_2+ d(O-O)= 1.440
  O      0.025008   -0.014506   -0.000000
  O      1.465008   -0.014439   -0.000000
  Pt     0.744902    1.761042   -0.000000
  O      0.745014    2.657420   -1.426913
  O      0.745014    2.657420    1.426913

  5
PtO4_2+ d(O-O)= 1.390
  O      0.024997   -0.015989    0.000000
  O      1.414997   -0.016007   -0.000000
  Pt     0.720005    1.780335   -0.000000
  O      0.720118    2.685481   -1.422501
  O      0.720118    2.685481    1.422501

  5
PtO4_2+ d(O-O)= 1.340
  O      0.024998   -0.018174   -0.000000
  O      1.364998   -0.018184   -0.000000
  Pt     0.695001    1.801972    0.000000
  O      0.695081    2.716838   -1.417864
  O      0.695081    2.716838    1.417864

  5
PtO4_2+ minimum C d(O-O)= 1.290
  O      0.024994   -0.021065   -0.000000
  O      1.314994   -0.021097   -0.000000
  Pt     0.670043    1.827013    0.000000
  O      0.670042    2.752667   -1.413035
  O      0.670042    2.752667    1.413035

  5
PtNO3+ minimum A d(O-O)=2.840
  Pt     0.000000    0.000061   -0.008240
  O     -1.419904   -0.819856    0.535873
  O      1.419904   -0.819856    0.535874
  O     -0.000000    1.639710    0.535935
  N     -0.000000   -0.000059   -1.706419

  5
PtNO3+ d(O-O)=2.800
  Pt     0.172647    0.052435   -0.038039
  O     -0.931507   -1.024392    0.687342
  O      1.593333   -0.737647    0.474133
  O      0.032223    1.685674    0.499185
  N      0.033307    0.023933   -1.729600

  5
PtNO3+ d(O-O)=2.750
  Pt     0.171302    0.060612   -0.042922
  O     -0.904813   -1.033187    0.692674
  O      1.570518   -0.752021    0.483674
  O      0.030924    1.693593    0.494116
  N      0.032071    0.031007   -1.734519

  5
PtNO3+ d(O-O)=2.700
  Pt     0.170001    0.068515   -0.047727
  O     -0.878159   -1.041690    0.697854
  O      1.547666   -0.766091    0.493123
  O      0.029677    1.701292    0.489163
  N      0.030817    0.037977   -1.739391

  5
PtNO3+ d(O-O)=2.650
  Pt     0.168735    0.076152   -0.052495
  O     -0.851542   -1.049938    0.702967
  O      1.524778   -0.779882    0.502529
  O      0.028481    1.708705    0.484235
  N      0.029549    0.044966   -1.744215

  5
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PtNO3+ d(O-O)=2.600

Pt	0.167516	0.083420	-0.057273
O	-0.824958	-1.057764	0.708103
O	1.501861	-0.793336	0.511917
O	0.027294	1.715840	0.479638
N	0.028290	0.051843	-1.749363

5

PtNO3+ d(O-O)=2.550

Pt	0.155149	0.250278	-0.148703
O	-0.794060	-1.209535	0.768608
O	1.483370	-0.943649	0.588014
O	0.021739	1.841126	0.490329
N	0.033803	0.061782	-1.805226

5

PtNO3+ d(O-O)=2.500

Pt	0.155149	0.250278	-0.148703
O	-0.794060	-1.209535	0.768608
O	1.483370	-0.943649	0.588014
O	0.021739	1.841126	0.490329
N	0.033803	0.061782	-1.805226

5

PtNO3+ d(O-O)=2.450

Pt	0.143052	0.253600	-0.149296
O	-0.763148	-1.207133	0.767872
O	1.467021	-0.962595	0.597446
O	0.019183	1.846905	0.483770
N	0.033894	0.069227	-1.806769

5

PtNO3+ d(O-O)=2.400

Pt	0.143052	0.253600	-0.149296
O	-0.763148	-1.207133	0.767872
O	1.467021	-0.962595	0.597446
O	0.019183	1.846905	0.483770
N	0.033894	0.069227	-1.806769

5

PtNO3+ d(O-O)=2.350

Pt	0.143052	0.253600	-0.149296
O	-0.763148	-1.207133	0.767872
O	1.467021	-0.962595	0.597446
O	0.019183	1.846905	0.483770
N	0.033894	0.069227	-1.806769

5

PtNO3+ d(O-O)=2.300

Pt	0.167509	0.090726	-0.061817
O	-0.813444	-1.055767	0.706843
O	1.467410	-0.823061	0.523675
O	0.044367	1.723066	0.478974
N	0.034160	0.065039	-1.754654

5

PtNO3+ TS B DFT(B3LYP)/ZORA d(O-O)=2.246

Pt	-0.021719	0.145455	-0.109088
O	-0.844472	-1.088104	0.798084
O	1.570703	-0.879317	0.490923
O	0.063398	1.759345	0.502703
N	0.132091	0.062624	-1.789599

5

PtNO3+ d(O-O)=2.200

Pt	0.142311	0.257524	-0.151139
O	-0.737002	-1.212231	0.770565
O	1.443682	-0.973450	0.604430
O	0.018217	1.851739	0.477787
N	0.032793	0.076421	-1.808621

5

PtNO3+ d(O-O)=2.155

Pt	0.141683	0.260991	-0.152456
O	-0.713743	-1.216860	0.773210
O	1.422584	-0.983116	0.610029
O	0.017215	1.856262	0.472307
N	0.032263	0.082725	-1.810068

5

PtNO3+ d(O-O)=2.108

Pt	0.141102	0.264669	-0.153810
O	-0.689145	-1.221447	0.775648
O	1.400236	-0.993062	0.615813
O	0.016190	1.860922	0.466869
N	0.031618	0.088922	-1.811497

5

PtNO3+ d(O-O)=2.061

Pt	0.140580	0.268266	-0.155141
O	-0.664620	-1.225871	0.777973
O	1.377790	-1.002670	0.621408
O	0.015235	1.865435	0.461671
N	0.031018	0.094843	-1.812889

5

PtNO3+ d(O-O)=2.013

Pt	0.140057	0.271781	-0.156429
O	-0.640125	-1.230107	0.780147
O	1.355313	-1.012060	0.626888
O	0.014324	1.869848	0.456654
N	0.030432	0.100540	-1.814237

5

PtNO3+ d(O-O)=1.966

Pt	0.139548	0.275228	-0.157672
O	-0.615641	-1.234199	0.782224
O	1.332832	-1.021364	0.632292
O	0.013408	1.874222	0.451729
N	0.029856	0.106116	-1.815551

5

PtNO3+ d(O-O)=1.918

Pt	0.139057	0.278617	-0.158877
O	-0.591167	-1.238170	0.784242
O	1.310351	-1.030626	0.637631
O	0.012468	1.878564	0.446855
N	0.029292	0.111617	-1.816829

5

PtNO3+ d(O-O)=1.871

Pt	0.138540	0.282135	-0.160165
O	-0.566725	-1.241957	0.786033
O	1.287839	-1.039659	0.642827
O	0.011594	1.882892	0.442421
N	0.028754	0.116592	-1.818094

5

PtNO3+ d(O-O)=1.824

Pt	0.138070	0.285477	-0.161428
O	-0.542281	-1.245694	0.787813
O	1.265337	-1.048654	0.648115
O	0.010726	1.887125	0.437881
N	0.028150	0.121749	-1.819358

5

PtNO3+ d(O-O)=1.776

Pt	0.137621	0.288797	-0.162753
O	-0.517840	-1.249358	0.789537
O	1.242843	-1.057594	0.653451
O	0.009873	1.891325	0.433454
N	0.027505	0.126834	-1.820666

5

PtNO3+ d(O-O)=1.729

Pt	0.137194	0.292116	-0.164137
O	-0.493392	-1.253019	0.791246
O	1.220366	-1.066556	0.658863
O	0.009018	1.895543	0.429073
N	0.026816	0.131919	-1.822024

5

PtNO3+ d(O-O)=1.682

Pt	0.136768	0.295444	-0.165582
O	-0.468936	-1.256746	0.793012
O	1.197894	-1.075561	0.664336

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  O      0.008164    1.899814    0.424699
  N      0.026112    0.137052   -1.823444

  5
PtNO3+ d(O-O)=1.634
  Pt     0.136311    0.298801   -0.167089
  O     -0.444465   -1.260635    0.794911
  O      1.175423   -1.084653    0.669866
  O      0.007312    1.904195    0.420281
  N      0.025421    0.142295   -1.824948

  5
PtNO3+ d(O-O)=1.587
  Pt     0.135817    0.302235   -0.168658
  O     -0.419958   -1.264802    0.796961
  O      1.152980   -1.093945    0.675542
  O      0.006456    1.908786    0.415735
  N      0.024707    0.147729   -1.826559

  5
PtNO3+ d(O-O)=1.539
  Pt     0.135310    0.305801   -0.170278
  O     -0.395392   -1.269349    0.799202
  O      1.130598   -1.103618    0.681446
  O      0.005549    1.913711    0.410948
  N      0.023938    0.153457   -1.828297

  5
PtNO3+ d(O-O)=1.492
  Pt     0.134791    0.309556   -0.171953
  O     -0.370749   -1.274380    0.801770
  O      1.108296   -1.113859    0.687590
  O      0.004529    1.919092    0.405826
  N      0.023136    0.159594   -1.830212

  5
PtNO3+ d(O-O)=1.445
  Pt     0.134247    0.313576   -0.173714
  O     -0.346008   -1.280111    0.804673
  O      1.086090   -1.124732    0.694137
  O      0.003437    1.925052    0.400311
  N      0.022237    0.166218   -1.832385

  5
PtNO3+ d(O-O)=1.397
  Pt     0.133570    0.317966   -0.175593
  O     -0.321127   -1.286759    0.808118
  O      1.064007   -1.136448    0.701119
  O      0.002258    1.931780    0.394306
  N      0.021295    0.173465   -1.834929

  5
PtNO3+ minimum C d(O-O)=1.351
  Pt    -0.021104    0.144159    0.000046
  O     -1.308472    1.280943    0.004743
  O     -0.077511   -1.678036   -0.675361
  O     -0.072832   -1.678117    0.675617
  N      1.493512    0.847490   -0.005044

  5
PtNO3+ minimum A d(N-O)=2.778
  Pt     0.000000    0.000061   -0.008240
  O     -1.419904   -0.819856    0.535873
  O      1.419904   -0.819856    0.535874
  O     -0.000000    1.639710    0.535935
  N     -0.000000   -0.000059   -1.706419

  5
PtNO3+ d(N-O)=2.745
  Pt     0.000000   -0.004910   -0.003897
  O     -1.419756   -0.823677    0.541166
  O      1.419756   -0.823677    0.541167
  O     -0.000000    1.639580    0.513044
  N      0.000000    0.012685   -1.698456

  5
PtNO3+ d(N-O)=2.691
  Pt    -0.000000   -0.013424    0.003203
  O     -1.419998   -0.832239    0.546294
  O      1.419998   -0.832239    0.546295
  O     -0.000000    1.636705    0.482054
  N      0.000001    0.041197   -1.684821

  5
PtNO3+ d(N-O)=2.636
  Pt    -0.000000   -0.021922    0.010084
  O     -1.420328   -0.840614    0.551378
  O      1.420328   -0.840614    0.551379
  O     -0.000000    1.633605    0.451238
  N      0.000000    0.069545   -1.671055

  5
PtNO3+ d(N-O)=2.582
  Pt    -0.000000   -0.030469    0.016728
  O     -1.420673   -0.848824    0.556518
  O      1.420673   -0.848823    0.556520
  O     -0.000000    1.630263    0.420560
  N      0.000001    0.097853   -1.657301

  5
PtNO3+ d(N-O)=2.527
  Pt    -0.000000   -0.039116    0.022929
  O     -1.421386   -0.856753    0.561561
  O      1.421386   -0.856753    0.561562
  O     -0.000000    1.626733    0.390169
  N      0.000001    0.125890   -1.643198

  5
PtNO3+ d(N-O)=2.473
  Pt    -0.000000   -0.047845    0.028841
  O     -1.421840   -0.864617    0.566792
  O      1.421840   -0.864617    0.566793
  O     -0.000000    1.623026    0.359847
  N      0.000000    0.154053   -1.629248

  5
PtNO3+ d(N-O)=2.418
  Pt     0.000000   -0.056808    0.034320
  O     -1.422324   -0.872333    0.572155
  O      1.422324   -0.872333    0.572156
  O     -0.000000    1.619206    0.329670
  N      0.000000    0.182268   -1.615276

  5
PtNO3+ d(N-O)=2.364
  Pt    -0.000000   -0.066281    0.039218
  O     -1.422903   -0.879856    0.577765
  O      1.422902   -0.879856    0.577766
  O     -0.000000    1.615302    0.299643
  N      0.000000    0.210690   -1.601368

  5
PtNO3+ d(N-O)=2.309
  Pt     0.000000   -0.076790    0.043351
  O     -1.423893   -0.887030    0.583690
  O      1.423893   -0.887030    0.583692
  O     -0.000000    1.611393    0.269813
  N      0.000000    0.239457   -1.587522

  5
PtNO3+ TS B' d(N-O)=2.247
  Pt    -0.000000   -0.183430    0.048770
  O     -1.453424   -0.906796    0.612276
  O      1.453424   -0.906795    0.612279
  O      0.000001    1.667710    0.212243
  N     -0.000001    0.329311   -1.592544

  5
PtNO3+ d(N-O)=2.150
  Pt     0.000000   -0.218120    0.132514
  O     -1.476954   -0.937934    0.602477
  O      1.476953   -0.937933    0.602478
  O      0.000000    1.701329    0.130696
  N      0.000001    0.392658   -1.575141

  5
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PtNO3+ d(N-O)=2.100

Pt	-0.000000	-0.219574	0.146312
O	-1.475730	-0.946740	0.604177
O	1.475729	-0.946740	0.604179
O	-0.000000	1.695725	0.102200
N	0.000000	0.417329	-1.563844

5

PtNO3+ d(N-O)=2.050

Pt	-0.000000	-0.220315	0.157722
O	-1.473474	-0.955493	0.606554
O	1.473474	-0.955492	0.606555
O	0.000000	1.689549	0.074347
N	0.000001	0.441751	-1.552153

5

PtNO3+ d(N-O)=2.000

Pt	-0.000000	-0.220744	0.167553
O	-1.470715	-0.964060	0.609236
O	1.470715	-0.964060	0.609238
O	-0.000000	1.683040	0.046970
N	0.000000	0.465824	-1.539973

5

PtNO3+ d(N-O)=1.950

Pt	-0.000000	-0.221047	0.176203
O	-1.467538	-0.972695	0.612110
O	1.467538	-0.972695	0.612111
O	-0.000000	1.676872	0.019735
N	0.000000	0.489565	-1.527134

5

PtNO3+ d(N-O)=1.900

Pt	-0.000000	-0.221313	0.183942
O	-1.463999	-0.981513	0.615142
O	1.463998	-0.981513	0.615143
O	-0.000000	1.671288	-0.007527
N	0.000000	0.513051	-1.513677

5

PtNO3+ d(N-O)=1.850

Pt	-0.000000	-0.222428	0.190806
O	-1.461192	-0.989589	0.618310
O	1.461191	-0.989589	0.618311
O	-0.000000	1.665147	-0.034302
N	0.000000	0.536459	-1.500101

5

PtNO3+ d(N-O)=1.800

Pt	-0.000000	-0.222522	0.197198
O	-1.456579	-0.998850	0.622020
O	1.456579	-0.998850	0.622021
O	-0.000000	1.659971	-0.061610
N	0.000000	0.560251	-1.486606

5

PtNO3+ d(N-O)=1.750

Pt	-0.000000	-0.223290	0.202899
O	-1.452486	-1.007869	0.625884
O	1.452486	-1.007869	0.625885
O	-0.000000	1.655010	-0.088818
N	0.000001	0.584018	-1.472825

5

PtNO3+ d(N-O)=1.700

Pt	0.000000	-0.224219	0.208519
O	-1.448613	-1.017166	0.629756
O	1.448612	-1.017165	0.629757
O	0.000000	1.650878	-0.116364
N	0.000001	0.607672	-1.458645

5

PtNO3+ d(N-O)=1.650

Pt	-0.000000	-0.225375	0.213721
O	-1.444408	-1.026682	0.633911
O	1.444407	-1.026682	0.633912
O	0.000000	1.647179	-0.144065
N	0.000001	0.631560	-1.444457

5

PtNO3+ d(N-O)=1.600

Pt	-0.000000	-0.226850	0.218779
O	-1.440222	-1.036500	0.638305
O	1.440221	-1.036500	0.638306
O	0.000000	1.644110	-0.172072
N	0.000000	0.655739	-1.430294

5

PtNO3+ d(N-O)=1.550

Pt	-0.000000	-0.228616	0.223944
O	-1.436042	-1.046882	0.642926
O	1.436042	-1.046882	0.642927
O	-0.000000	1.642149	-0.200683
N	0.000000	0.680231	-1.416090

5

PtNO3+ d(N-O)=1.500

Pt	0.000000	-0.230607	0.229498
O	-1.431793	-1.058163	0.647784
O	1.431792	-1.058163	0.647785
O	0.000000	1.641849	-0.230259
N	0.000000	0.705085	-1.401785

5

PtNO3+ d(N-O)=1.450

Pt	-0.000000	-0.232825	0.235855
O	-1.427613	-1.070472	0.652783
O	1.427612	-1.070472	0.652784
O	-0.000000	1.643488	-0.261048
N	0.000000	0.730282	-1.387350

5

PtNO3+ d(N-O)=1.400

Pt	-0.000000	-0.235251	0.243510
O	-1.423551	-1.084135	0.657848
O	1.423550	-1.084135	0.657849
O	-0.000000	1.647718	-0.293534
N	0.000000	0.755804	-1.372649

5

PtNO3+ d(N-O)=1.350

Pt	-0.000000	-0.238031	0.252917
O	-1.419717	-1.099473	0.662993
O	1.419716	-1.099472	0.662994
O	0.000000	1.655181	-0.328232
N	0.000000	0.781795	-1.357649

5

PtNO3+ d(N-O)=1.300

Pt	-0.000000	-0.241305	0.264395
O	-1.417020	-1.116272	0.668015
O	1.417020	-1.116272	0.668016
O	0.000000	1.665746	-0.365222
N	0.000000	0.808102	-1.342180

5

PtNO3+ minimum C' d(N-O)=1.196

Pt	-0.113467	-0.125598	0.000000
O	0.048978	-1.086796	-1.418614
O	0.048980	-1.086797	1.418614
O	-0.514583	1.931090	-0.000002
N	0.653617	1.674886	0.000001

5

PtN2O2 minimum A d(O-O)=2.900

Pt	-0.728007	0.263451	-0.161463
O	-0.136982	1.075575	1.287341
O	-0.162404	1.090073	-1.612200
N	-0.157262	-1.354142	-0.174577
N	-2.443308	0.259655	-0.146557

5

PtN2O2 d(O-O)=2.890

Pt	-0.007732	-0.000088	0.175902
O	1.407848	0.001247	1.224833
O	-1.480957	0.009024	1.142093

```
  N      0.016429   -1.404151   -0.808843
  N      0.024374    1.393709   -0.823092

  5
PtN2O2 d(O-O)=2.840
  Pt    -0.007435   -0.000142    0.165496
  O      1.382424    0.001396    1.239603
  O     -1.456401    0.009035    1.158276
  N      0.016713   -1.403953   -0.819118
  N      0.024661    1.393405   -0.833365

  5
PtN2O2 d(O-O)=2.790
  Pt    -0.007188   -0.000198    0.155222
  O      1.356964    0.001540    1.254069
  O     -1.431885    0.009053    1.174308
  N      0.017067   -1.403810   -0.829232
  N      0.025004    1.393156   -0.843473

  5
PtN2O2 d(O-O)=2.740
  Pt    -0.006912   -0.000256    0.145107
  O      1.331540    0.001677    1.268335
  O     -1.407331    0.009082    1.190034
  N      0.017378   -1.403713   -0.839177
  N      0.025288    1.392951   -0.853406

  5
PtN2O2 d(O-O)=2.690
  Pt    -0.006623   -0.000309    0.135171
  O      1.306140    0.001814    1.282347
  O     -1.382750    0.009099    1.205438
  N      0.017650   -1.403660   -0.848918
  N      0.025544    1.392796   -0.863144

  5
PtN2O2 d(O-O)=2.640
  Pt    -0.006365   -0.000358    0.125437
  O      1.280733    0.001950    1.295966
  O     -1.358179    0.009111    1.220526
  N      0.017945   -1.403660   -0.858405
  N      0.025828    1.392698   -0.872632

  5
PtN2O2 d(O-O)=2.590
  Pt    -0.006142   -0.000405    0.115892
  O      1.255310    0.002086    1.309246
  O     -1.333627    0.009116    1.235380
  N      0.018271   -1.403685   -0.867697
  N      0.026150    1.392628   -0.881928

  5
PtN2O2 d(O-O)=2.540
  Pt    -0.005934   -0.000450    0.106557
  O      1.229903    0.002236    1.322233
  O     -1.309058    0.009105    1.249920
  N      0.018574   -1.403712   -0.876790
  N      0.026477    1.392562   -0.891027

  5
PtN2O2 d(O-O)=2.490
  Pt    -0.005678   -0.000491    0.097458
  O      1.204522    0.002387    1.334978
  O     -1.284461    0.009083    1.264115
  N      0.018820   -1.403746   -0.885705
  N      0.026759    1.392508   -0.899953

  5
PtN2O2 d(O-O)=2.440
  Pt    -0.005360   -0.000532    0.088537
  O      1.179190    0.002530    1.347560
  O     -1.259807    0.009066    1.277938
  N      0.018989   -1.403715   -0.894442
  N      0.026950    1.392392   -0.908700

  5
PtN2O2 d(O-O)=2.390
  Pt    -0.004996   -0.000581    0.080033
  O      1.153859    0.002668    1.359788
  O     -1.235153    0.009069    1.291394
  N      0.019145   -1.403917   -0.903036
  N      0.027107    1.392501   -0.917286

  5
PtN2O2 d(O-O)=2.340
  Pt    -0.151887   -0.000862   -0.061885
  O      1.157835    0.003393    1.486582
  O     -1.181493    0.009498    1.430843
  N      0.063584   -1.435891   -0.965016
  N      0.071923    1.423602   -0.979631

  5
PtN2O2 TS B d(O-O)=2.310
  Pt     0.001866    0.149772   -0.135334
  O     -0.774520   -1.081836    0.890145
  O      1.492903   -0.934046    0.494395
  N      0.014057    1.739906    0.489247
  N      0.165695    0.126207   -1.845430

  5
PtN2O2 d(O-O)=2.290
  Pt    -0.127372   -0.001032   -0.083251
  O      1.136084    0.003698    1.532289
  O     -1.152207    0.009454    1.444011
  N      0.047529   -1.440162   -0.983737
  N      0.055928    1.427783   -0.998419

  5
PtN2O2 d(O-O)=2.240
  Pt    -0.100915   -0.001203   -0.097982
  O      1.110629    0.003899    1.564465
  O     -1.126819    0.009524    1.457730
  N      0.034370   -1.442002   -0.999332
  N      0.042698    1.429524   -1.013988

  5
PtN2O2 d(O-O)=2.190
  Pt    -0.014187   -0.001527   -0.116116
  O      1.061912    0.004049    1.571753
  O     -1.127100    0.009740    1.506199
  N      0.015489   -1.445657   -1.018084
  N      0.023848    1.433135   -1.032860

  5
PtN2O2 d(O-O)=2.140
  Pt    -0.002568   -0.001550   -0.120744
  O      1.031737    0.004150    1.573504
  O     -1.107677    0.009743    1.523743
  N      0.015045   -1.443643   -1.025416
  N      0.023425    1.431042   -1.040194

  5
PtN2O2 d(O-O)=2.090
  Pt    -0.001627   -0.001577   -0.125244
  O      1.006217    0.004292    1.581120
  O     -1.083233    0.009694    1.533448
  N      0.015093   -1.441880   -1.031838
  N      0.023511    1.429212   -1.046592

  5
PtN2O2 d(O-O)=2.040
  Pt    -0.001282   -0.001601   -0.129610
  O      0.980972    0.004462    1.588714
  O     -1.058493    0.009611    1.542309
  N      0.015132   -1.440347   -1.037894
  N      0.023633    1.427616   -1.052626

  5
PtN2O2 d(O-O)=1.990
  Pt    -0.001060   -0.001629   -0.133843
  O      0.955780    0.004607    1.595987
  O     -1.033699    0.009556    1.550727
  N      0.015197   -1.438998   -1.043638
  N      0.023744    1.426205   -1.058341

  5
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PtN2O2 d(O-O)=1.940

Pt	-0.000884	-0.001665	-0.138011
O	0.930590	0.004695	1.603035
O	-1.008904	0.009569	1.558978
N	0.015328	-1.437750	-1.049225
N	0.023832	1.424891	-1.063884

5

PtN2O2 d(O-O)=1.890

Pt	-0.000767	-0.001699	-0.142093
O	0.905406	0.004758	1.609721
O	-0.984104	0.009604	1.566927
N	0.015499	-1.436712	-1.054522
N	0.023928	1.423791	-1.069140

5

PtN2O2 d(O-O)=1.840

Pt	-0.000702	-0.001732	-0.146109
O	0.880220	0.004808	1.616044
O	-0.959308	0.009646	1.574617
N	0.015705	-1.435854	-1.059539
N	0.024047	1.422874	-1.074121

5

PtN2O2 d(O-O)=1.790

Pt	-0.000635	-0.001761	-0.150100
O	0.855056	0.004851	1.622166
O	-0.934487	0.009685	1.582001
N	0.015887	-1.435174	-1.064309
N	0.024141	1.422139	-1.078865

5

PtN2O2 d(O-O)=1.740

Pt	-0.000543	-0.001786	-0.154105
O	0.829902	0.004901	1.628186
O	-0.909655	0.009712	1.589215
N	0.016039	-1.434643	-1.068931
N	0.024218	1.421557	-1.083472

5

PtN2O2 d(O-O)=1.690

Pt	-0.000447	-0.001807	-0.158147
O	0.804747	0.004967	1.634123
O	-0.884825	0.009714	1.596365
N	0.016178	-1.434246	-1.073456
N	0.024309	1.421113	-1.087992

5

PtN2O2 d(O-O)=1.640

Pt	-0.000346	-0.001825	-0.162256
O	0.779604	0.005036	1.640060
O	-0.859980	0.009706	1.603430
N	0.016296	-1.433995	-1.077899
N	0.024387	1.420819	-1.092443

5

PtN2O2 d(O-O)=1.590

Pt	-0.000228	-0.001839	-0.166484
O	0.754469	0.005122	1.646091
O	-0.835127	0.009675	1.610516
N	0.016386	-1.433888	-1.082335
N	0.024461	1.420670	-1.096896

5

PtN2O2 d(O-O)=1.540

Pt	-0.000252	-0.001853	-0.170896
O	0.729322	0.005218	1.652217
O	-0.810290	0.009636	1.617925
N	0.016556	-1.433909	-1.086887
N	0.024626	1.420649	-1.101467

5

PtN2O2 d(O-O)=1.490

Pt	0.000186	-0.001870	-0.175541
O	0.704119	0.005329	1.658822
O	-0.785504	0.009587	1.625590
N	0.016540	-1.434066	-1.091689
N	0.024621	1.420761	-1.106289

5

PtN2O2 d(O-O)=1.440

Pt	-0.000493	-0.001887	-0.180584
O	0.679006	0.005483	1.665670
O	-0.760643	0.009503	1.634171
N	0.016978	-1.434328	-1.096875
N	0.025114	1.420971	-1.111490

5

PtN2O2 minimum C d(O-O)=1.400

Pt	-0.000244	-0.001907	-0.184848
O	0.658345	0.005584	1.672109
O	-0.740275	0.009467	1.641312
N	0.016993	-1.434837	-1.101527
N	0.025143	1.421434	-1.116153

5

PtN2O2 minimum A d(N-O)=2.836

Pt	-0.728007	0.263451	-0.161463
O	-0.136982	1.075575	1.287341
O	-0.162404	1.090073	-1.612200
N	-0.157262	-1.354142	-0.174577
N	-2.443308	0.259655	-0.146557

5

PtN2O2 d(N-O)=2.825

Pt	-0.729230	0.264707	-0.160291
O	-0.172419	0.964668	1.358787
O	-0.040116	1.124361	-1.534944
N	-0.245772	-1.378069	-0.239281
N	-2.440428	0.358947	-0.231729

5

PtN2O2 d(N-O)=2.771

Pt	-0.734917	0.270243	-0.152119
O	-0.178399	0.968806	1.367059
O	-0.032966	1.093734	-1.534466
N	-0.235544	-1.360173	-0.263544
N	-2.446139	0.362003	-0.224387

5

PtN2O2 d(N-O)=2.716

Pt	-0.740587	0.275626	-0.143987
O	-0.184189	0.972896	1.375239
O	-0.025905	1.063234	-1.533858
N	-0.225446	-1.342122	-0.287633
N	-2.451838	0.364980	-0.217218

5

PtN2O2 d(N-O)=2.662

Pt	-0.746252	0.280829	-0.135896
O	-0.189771	0.976940	1.383292
O	-0.018925	1.032878	-1.533092
N	-0.215487	-1.323906	-0.311532
N	-2.457529	0.367871	-0.210230

5

PtN2O2 d(N-O)=2.607

Pt	-0.751907	0.285800	-0.127813
O	-0.195191	0.980988	1.391220
O	-0.012033	1.002657	-1.532169
N	-0.205636	-1.305563	-0.335294
N	-2.463197	0.370730	-0.203401

5

PtN2O2 d(N-O)=2.553

Pt	-0.757544	0.290470	-0.119695
O	-0.200483	0.985114	1.399023
O	-0.005233	0.972571	-1.531082
N	-0.195887	-1.287132	-0.358986
N	-2.468817	0.373590	-0.196717

5

PtN2O2 d(N-O)=2.498

Pt	-0.763215	0.294702	-0.111435
O	-0.205688	0.989485	1.406654
O	0.001543	0.942626	-1.529781
N	-0.186185	-1.268715	-0.382768

```
  N     -2.474419    0.376515   -0.190127

  5
PtN2O2 d(N-O)=2.444
  Pt    -0.768982    0.298366   -0.102890
  O     -0.210770    0.994150    1.414117
  O      0.008243    0.912827   -1.528275
  N     -0.176431   -1.250345   -0.406696
  N     -2.480025    0.379615   -0.183713

  5
PtN2O2 d(N-O)=2.389
  Pt    -0.774948    0.301353   -0.093827
  O     -0.215683    0.999142    1.421497
  O      0.014905    0.883167   -1.526738
  N     -0.166573   -1.231974   -0.430838
  N     -2.485667    0.382924   -0.177552

  5
PtN2O2 d(N-O)=2.335
  Pt    -0.781343    0.303542   -0.083801
  O     -0.220426    1.004549    1.428913
  O      0.021847    0.853596   -1.525568
  N     -0.156499   -1.213544   -0.455416
  N     -2.491544    0.386470   -0.171584

5
PtN2O2 TS B' d(N-O)=2.280
  Pt    -0.831188    0.294158    0.005005
  O     -0.220622    1.029340    1.475125
  O      0.056984    0.805580   -1.592373
  N     -0.112029   -1.202449   -0.521094
  N     -2.521110    0.407984   -0.174120

  5
PtN2O2 d(N-O)=2.228
  Pt    -0.859649    0.342080    0.038677
  O     -0.224326    1.023056    1.518183
  O      0.084981    0.754275   -1.640306
  N     -0.089165   -1.185167   -0.558643
  N     -2.539806    0.400368   -0.165368

  5
PtN2O2 d(N-O)=2.175
  Pt    -0.865558    0.358512    0.042313
  O     -0.230155    1.020901    1.529020
  O      0.090071    0.722607   -1.641190
  N     -0.077729   -1.168423   -0.579836
  N     -2.544595    0.401016   -0.157765

  5
PtN2O2 d(N-O)=2.123
  Pt    -0.869845    0.372288    0.044377
  O     -0.236135    1.019115    1.537887
  O      0.093392    0.692242   -1.639200
  N     -0.066939   -1.151487   -0.599987
  N     -2.548439    0.402455   -0.150534

  5
PtN2O2 d(N-O)=2.070
  Pt    -0.873307    0.383885    0.045815
  O     -0.242295    1.017897    1.545424
  O      0.096158    0.662792   -1.635624
  N     -0.056780   -1.134307   -0.619776
  N     -2.551741    0.404346   -0.143297

  5
PtN2O2 d(N-O)=2.018
  Pt    -0.876329    0.393911    0.046972
  O     -0.248432    1.017154    1.552035
  O      0.098689    0.634011   -1.630963
  N     -0.047131   -1.116934   -0.639381
  N     -2.554762    0.406471   -0.136120

  5
PtN2O2 d(N-O)=1.965
  Pt    -0.879024    0.402744    0.048031
  O     -0.254765    1.016637    1.558223
  O      0.101418    0.605574   -1.626219
  N     -0.038001   -1.099058   -0.658740
  N     -2.557592    0.408716   -0.128753

  5
PtN2O2 d(N-O)=1.913
  Pt    -0.881436    0.410689    0.049073
  O     -0.261395    1.016130    1.564353
  O      0.104630    0.577245   -1.622102
  N     -0.029474   -1.080399   -0.677703
  N     -2.560290    0.410948   -0.121078

  5
PtN2O2 d(N-O)=1.860
  Pt    -0.883740    0.417930    0.050293
  O     -0.267837    1.015880    1.570363
  O      0.107859    0.549115   -1.617911
  N     -0.021295   -1.061482   -0.696556
  N     -2.562952    0.413169   -0.113646

  5
PtN2O2 d(N-O)=1.808
  Pt    -0.886046    0.424470    0.051512
  O     -0.273963    1.015892    1.576210
  O      0.111200    0.521226   -1.613445
  N     -0.013253   -1.042434   -0.715373
  N     -2.565903    0.415458   -0.106361

  5
PtN2O2 d(N-O)=1.755
  Pt    -0.888332    0.430948    0.052706
  O     -0.280485    1.015746    1.581914
  O      0.115066    0.493257   -1.609486
  N     -0.005599   -1.022979   -0.733989
  N     -2.568614    0.417641   -0.098602

  5
PtN2O2 d(N-O)=1.703
  Pt    -0.890575    0.437011    0.053988
  O     -0.287135    1.015660    1.587890
  O      0.119391    0.465172   -1.606237
  N      0.001799   -1.003065   -0.752446
  N     -2.571447    0.419835   -0.090653

  5
PtN2O2 d(N-O)=1.650
  Pt    -0.892870    0.442468    0.055585
  O     -0.294519    1.015864    1.594003
  O      0.124168    0.436901   -1.603680
  N      0.009498   -0.983149   -0.771330
  N     -2.574243    0.422529   -0.082034

  5
PtN2O2 d(N-O)=1.598
  Pt    -0.895223    0.447895    0.057247
  O     -0.301934    1.016251    1.600542
  O      0.129471    0.408445   -1.601645
  N      0.017105   -0.963143   -0.790395
  N     -2.577385    0.425165   -0.073206

  5
PtN2O2 d(N-O)=1.545
  Pt    -0.897787    0.453385    0.059116
  O     -0.309486    1.016629    1.607495
  O      0.135507    0.379620   -1.600569
  N      0.024786   -0.942870   -0.809502
  N     -2.580985    0.427848   -0.063996

  5
PtN2O2 d(N-O)=1.493
  Pt    -0.900582    0.459136    0.061232
  O     -0.317406    1.016941    1.615180
  O      0.142371    0.350157   -1.600962
  N      0.032733   -0.922291   -0.828686
  N     -2.585082    0.430670   -0.054220

  5
PtN2O2 d(N-O)=1.440
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  Pt    -0.903783    0.465375    0.063618
  O     -0.325588    1.017144    1.623658
  O      0.150250    0.319936   -1.602916
  N      0.041085   -0.901455   -0.848008
  N     -2.589929    0.433613   -0.043808

  5
PtN2O2 d(N-O)=1.388
  Pt    -0.907541    0.472389    0.066397
  O     -0.334048    1.017156    1.633216
  O      0.159464    0.288638   -1.606991
  N      0.049931   -0.880218   -0.867441
  N     -2.595771    0.436648   -0.032637

  5
PtN2O2 d(N-O)=1.335
  Pt    -0.912043    0.480335    0.069463
  O     -0.342204    1.016922    1.644094
  O      0.170140    0.256141   -1.613236
  N      0.059256   -0.858398   -0.886784
  N     -2.603113    0.439613   -0.020994

  5
PtN2O2 d(N-O)=1.283
  Pt    -0.918140    0.489839    0.073457
  O     -0.349686    1.016078    1.655945
  O      0.182672    0.222092   -1.621968
  N      0.069547   -0.835934   -0.906014
  N     -2.612357    0.442537   -0.008876

  5
PtN2O2 minimum C' d(N-O)=1.262
  Pt     0.020660    0.153568    0.091624
  O     -1.321519    1.286346   -0.068783
  O     -0.065797   -1.823972    0.628655
  N      1.524641    0.931708   -0.035617
  N     -0.144392   -1.631211   -0.615878

   5
PtN2O2 minimum A d(N-N)=2.798
  Pt    -0.728007    0.263451   -0.161463
  O     -0.136982    1.075575    1.287341
  O     -0.162404    1.090073   -1.612200
  N     -0.157262   -1.354142   -0.174577
  N     -2.443308    0.259655   -0.146557

  5
PtN2O2 d(N-N)=2.774
  Pt    -0.611656    0.160711    0.000010
  O     -0.015573   -1.497983   -0.009556
  O     -0.038185    1.018568    1.428971
  N     -2.323519    0.152574   -0.012493
  N     -0.070068    0.970129   -1.407931

  5
PtN2O2 d(N-N)=2.718
  Pt    -0.605743    0.156664    0.007164
  O     -0.009537   -1.501719   -0.001971
  O     -0.032144    1.014014    1.436069
  N     -2.309659    0.167025   -0.037556
  N     -0.101917    0.968015   -1.404706

  5
PtN2O2 d(N-N)=2.661
  Pt    -0.599893    0.152639    0.014226
  O     -0.003594   -1.505513    0.005491
  O     -0.026180    1.009610    1.443068
  N     -2.295683    0.181391   -0.062479
  N     -0.133650    0.965872   -1.401306

  5
PtN2O2 d(N-N)=2.605
  Pt    -0.594066    0.148655    0.021246
  O      0.002273   -1.509206    0.012897
  O     -0.020293    1.005196    1.449992
  N     -2.281609    0.195696   -0.087297
  N     -0.165305    0.963659   -1.397837

  5
PtN2O2 d(N-N)=2.549
  Pt    -0.588388    0.144776    0.028124
  O      0.008038   -1.513243    0.019894
  O     -0.014503    1.001302    1.457051
  N     -2.267369    0.209872   -0.111913
  N     -0.196778    0.961293   -1.394156

  5
PtN2O2 d(N-N)=2.493
  Pt    -0.582782    0.140938    0.034969
  O      0.013756   -1.516907    0.026958
  O     -0.008743    0.997155    1.463866
  N     -2.253076    0.223990   -0.136446
  N     -0.228154    0.958823   -1.390347

  5
PtN2O2 d(N-N)=2.436
  Pt    -0.577288    0.137141    0.041709
  O      0.019444   -1.520516    0.033951
  O     -0.003036    0.993040    1.470569
  N     -2.238705    0.238058   -0.160856
  N     -0.259416    0.956275   -1.386373

  5
PtN2O2 d(N-N)=2.380
  Pt    -0.571879    0.133401    0.048291
  O      0.025152   -1.524185    0.041000
  O      0.002665    0.988914    1.477281
  N     -2.224282    0.252116   -0.185206
  N     -0.290656    0.953753   -1.382366

  5
PtN2O2 TS B" d(N-N)=2.350
  Pt    -0.633628    0.054814    0.185419
  O      0.094012   -1.541568    0.064373
  O      0.071241    0.979187    1.504978
  N     -2.250162    0.311462   -0.289258
  N     -0.340304    1.001020   -1.465510

  5
PtN2O2 d(N-N)=2.346
  Pt    -0.463707    0.059377    0.179498
  O      0.052972   -1.595928    0.043903
  O      0.029479    1.023175    1.540814
  N     -2.291722    0.312967   -0.292628
  N     -0.386022    1.004408   -1.472587

  5
PtN2O2 d(N-N)=2.304
  Pt    -0.461402    0.057773    0.182305
  O      0.057237   -1.596698    0.050437
  O      0.033851    1.018031    1.544731
  N     -2.280419    0.322755   -0.309687
  N     -0.408267    1.002139   -1.468785

  5
PtN2O2 d(N-N)=2.263
  Pt    -0.459219    0.056261    0.184964
  O      0.061438   -1.597399    0.056883
  O      0.038155    1.012917    1.548573
  N     -2.268991    0.332461   -0.326588
  N     -0.430383    0.999759   -1.464832

  5
PtN2O2 d(N-N)=2.222
  Pt    -0.457140    0.054830    0.187496
  O      0.065583   -1.598026    0.063249
  O      0.042388    1.007824    1.552346
  N     -2.257450    0.342099   -0.343342
  N     -0.452381    0.997272   -1.460750

  5
PtN2O2 d(N-N)=2.180
  Pt    -0.455140    0.053461    0.189936
  O      0.069686   -1.598604    0.069537
  O      0.046558    1.002760    1.556071
  N     -2.245818    0.351689   -0.359975
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  N     -0.474287    0.994694   -1.456569
  5
PtN2O2 d(N-N)=2.139
  Pt    -0.453210    0.052148    0.192290
  O      0.073759   -1.599117    0.075780
  O      0.050676    0.997687    1.559755
  N     -2.234106    0.361245   -0.376504
  N     -0.496119    0.992036   -1.452321
  5
PtN2O2 d(N-N)=2.098
  Pt    -0.451333    0.050879    0.194576
  O      0.077833   -1.599617    0.082012
  O      0.054771    0.992605    1.563447
  N     -2.222348    0.370793   -0.392975
  N     -0.517922    0.989340   -1.448060
  5
PtN2O2 d(N-N)=2.057
  Pt    -0.449513    0.049648    0.196784
  O      0.081890   -1.600029    0.088267
  O      0.058828    0.987455    1.567072
  N     -2.210528    0.380317   -0.409369
  N     -0.539678    0.986609   -1.443754
  5
PtN2O2 d(N-N)=2.015
  Pt    -0.447731    0.048436    0.198939
  O      0.086008   -1.600517    0.094573
  O      0.062929    0.982300    1.570773
  N     -2.198738    0.389873   -0.425796
  N     -0.561468    0.983907   -1.439488
  5
PtN2O2 d(N-N)=1.974
  Pt    -0.445962    0.047230    0.201080
  O      0.090114   -1.600789    0.101000
  O      0.067035    0.976938    1.574331
  N     -2.186942    0.399411   -0.442218
  N     -0.583244    0.981209   -1.435193
  5
PtN2O2 d(N-N)=1.933
  Pt    -0.444240    0.046054    0.203179
  O      0.094343   -1.601459    0.107423
  O      0.071301    0.971795    1.578219
  N     -2.175271    0.409000   -0.458807
  N     -0.605133    0.978608   -1.431015
  5
PtN2O2 d(N-N)=1.891
  Pt    -0.442683    0.044984    0.205079
  O      0.098874   -1.601335    0.114812
  O      0.075898    0.965428    1.581898
  N     -2.163838    0.418742   -0.475685
  N     -0.627252    0.976180   -1.427104
    5
PtN2O2 d(N-N)=1.850
  Pt    -0.440891    0.043748    0.207265
  O      0.103054   -1.602205    0.121052
  O      0.080116    0.960553    1.585827
  N     -2.152159    0.428316   -0.492263
  N     -0.649120    0.973588   -1.422881
  5
PtN2O2 d(N-N)=1.850
  Pt    -0.440890    0.043745    0.207267
  O      0.103012   -1.601834    0.121201
  O      0.080085    0.960238    1.585590
  N     -2.151947    0.428352   -0.492331
  N     -0.649260    0.973498   -1.422728
  5
PtN2O2 d(N-N)=1.797
  Pt    -0.438694    0.042206    0.209951
  O      0.108732   -1.602392    0.130150
  O      0.085883    0.952912    1.590572
  N     -2.137268    0.440843   -0.514019
  N     -0.677654    0.970430   -1.417654
  5
PtN2O2 d(N-N)=1.743
  Pt    -0.436393    0.040630    0.212694
  O      0.114662   -1.602959    0.139445
  O      0.091849    0.945282    1.595771
  N     -2.122792    0.453525   -0.535950
  N     -0.706326    0.967521   -1.412961
  5
PtN2O2 d(N-N)=1.690
  Pt    -0.433900    0.038941    0.215629
  O      0.120873   -1.603807    0.149048
  O      0.098076    0.937529    1.601375
  N     -2.108668    0.466467   -0.558306
  N     -0.735381    0.964868   -1.408746
  5
PtN2O2 d(N-N)=1.637
  Pt    -0.431325    0.037149    0.218760
  O      0.127412   -1.604678    0.159125
  O      0.104688    0.929397    1.607233
  N     -2.094992    0.479657   -0.581208
  N     -0.764784    0.962474   -1.404910
  5
PtN2O2 d(N-N)=1.584
  Pt    -0.428507    0.035174    0.222244
  O      0.134404   -1.605825    0.169602
  O      0.111673    0.921024    1.613623
  N     -2.081876    0.493310   -0.604729
  N     -0.794694    0.960315   -1.401740
  5
PtN2O2 d(N-N)=1.531
  Pt    -0.425280    0.032947    0.226181
  O      0.141741   -1.607462    0.180543
  O      0.119119    0.912547    1.620608
  N     -2.069333    0.507248   -0.629031
  N     -0.825247    0.958720   -1.399301
  5
PtN2O2 d(N-N)=1.478
  Pt    -0.421441    0.030351    0.230807
  O      0.149305   -1.609885    0.191305
  O      0.126695    0.904578    1.628281
  N     -2.057255    0.521606   -0.653842
  N     -0.856304    0.957348   -1.397550
  5
PtN2O2 d(N-N)=1.425
  Pt    -0.416998    0.027315    0.236235
  O      0.157512   -1.613024    0.202712
  O      0.134995    0.896447    1.636879
  N     -2.046198    0.536573   -0.679929
  N     -0.888310    0.956688   -1.396897
  5
PtN2O2 d(N-N)=1.372
  Pt    -0.411670    0.023823    0.242514
  O      0.166484   -1.616946    0.214967
  O      0.144017    0.887961    1.646660
  N     -2.036274    0.552369   -0.707350
  N     -0.921557    0.956792   -1.397791
  5
PtN2O2 d(N-N)=1.319
  Pt    -0.405734    0.019313    0.250504
  O      0.176312   -1.622241    0.227236
  O      0.153821    0.880189    1.657561
  N     -2.027634    0.569117   -0.736388
  N     -0.955765    0.957622   -1.399914
  5
PtN2O2 d(N-N)=1.266
  Pt    -0.396951    0.014137    0.259619
```

```
  O      0.186329   -1.629253    0.240238
  O      0.163902    0.872738    1.670143
  N     -2.020348    0.586494   -0.766941
  N     -0.991932    0.959883   -1.404059

  5
PtN2O2 d(N-N)=1.213
  Pt    -0.386515    0.007558    0.271242
  O      0.197232   -1.639045    0.252652
  O      0.174752    0.867173    1.684918
  N     -2.014801    0.605201   -0.799583
  N     -1.029668    0.963112   -1.410230

  5
PtN2O2 minimum C" d(N-N)=1.160
  Pt     0.013901   -0.148359    0.000001
  O     -0.011931   -1.128621   -1.448815
  O     -0.011929   -1.128620    1.448815
  N     -0.511393    1.871474   -0.000001
  N      0.644878    1.840911    0.000001
  5
PtN3O- minimum A d(N-O)=2.889
  Pt    -0.000000    0.000050    0.008205
  N     -1.433251   -0.827594    0.563299
  N      1.433251   -0.827593    0.563299
  N      0.000000    1.655137    0.563285
  O     -0.000000    0.000001   -1.805065

  5
PtN3O- d(N-O)=2.850
  Pt     0.000000   -0.007099    0.011972
  N     -1.433073   -0.839824    0.559013
  N      1.433076   -0.839819    0.559013
  N     -0.000003    1.646478    0.558648
  O      0.000000    0.040264   -1.795620

  5
PtN3O- d(N-O)=2.800
  Pt    -0.000000   -0.015550    0.016782
  N     -1.433137   -0.847247    0.564928
  N      1.433139   -0.847242    0.564929
  N     -0.000003    1.643696    0.529908
  O      0.000000    0.066343   -1.783522

  5
PtN3O- d(N-O)=2.750
  Pt     0.000000   -0.023709    0.021628
  N     -1.433457   -0.854594    0.570651
  N      1.433460   -0.854589    0.570651
  N     -0.000003    1.640766    0.501293
  O      0.000000    0.092126   -1.771198

  5
PtN3O- d(N-O)=2.700
  Pt     0.000000   -0.031877    0.026782
  N     -1.433708   -0.861869    0.576256
  N      1.433711   -0.861865    0.576256
  N     -0.000003    1.637760    0.472648
  O      0.000000    0.117851   -1.758916

  5
PtN3O- d(N-O)=2.650
  Pt    -0.000000   -0.039888    0.032187
  N     -1.434027   -0.869125    0.581717
  N      1.434030   -0.869121    0.581718
  N     -0.000003    1.634691    0.443996
  O      0.000000    0.143444   -1.746593

  5
PtN3O- d(N-O)=2.600
  Pt     0.000000   -0.047706    0.037905
  N     -1.434416   -0.876383    0.586990
  N      1.434418   -0.876378    0.586991
  N     -0.000003    1.631602    0.415326
  O      0.000000    0.168865   -1.734186

  5
PtN3O- d(N-O)=2.550
  Pt     0.000000   -0.055315    0.044036
  N     -1.434885   -0.883666    0.592057
  N      1.434888   -0.883661    0.592058
  N     -0.000003    1.628515    0.386599
  O      0.000000    0.194127   -1.721725

  5
PtN3O- d(N-O)=2.500
  Pt     0.000000   -0.062739    0.050697
  N     -1.435445   -0.890999    0.596970
  N      1.435448   -0.890995    0.596971
  N     -0.000003    1.625399    0.357753
  O     -0.000000    0.219334   -1.709366

  5
PtN3O- d(N-O)=2.450
  Pt     0.000000   -0.069982    0.058181
  N     -1.436132   -0.898473    0.601715
  N      1.436134   -0.898468    0.601715
  N     -0.000003    1.622342    0.328658
  O     -0.000000    0.244581   -1.697243

  5
PtN3O- d(N-O)=2.400
  Pt     0.000000   -0.077037    0.067173
  N     -1.437032   -0.906302    0.606204
  N      1.437035   -0.906297    0.606204
  N     -0.000003    1.619613    0.299018
  O     -0.000000    0.270022   -1.685574
    5
PtN3O- d(N-O)=2.350
  Pt    -0.000000   -0.117443    0.166245
  N     -1.457423   -0.942845    0.621488
  N      1.457426   -0.942839    0.621489
  N     -0.000002    1.650770    0.221267
  O     -0.000001    0.352357   -1.737464

  5
PtN3O- TS B' d(N-O)=2.352
  Pt    -0.000002   -0.116223    0.165378
  N     -1.457066   -0.942268    0.621000
  N      1.457067   -0.942258    0.621000
  N      0.000001    1.650150    0.222937
  O     -0.000000    0.350599   -1.737290

  5
PtN3O- d(N-O)=2.300
  Pt     0.000000   -0.161961    0.183400
  N     -1.467391   -0.954052    0.646420
  N      1.467393   -0.954048    0.646421
  N     -0.000003    1.654365    0.177374
  O     -0.000000    0.415697   -1.760590

  5
PtN3O- d(N-O)=2.250
  Pt     0.000000   -0.181147    0.181499
  N     -1.468615   -0.959405    0.658298
  N      1.468617   -0.959400    0.658299
  N     -0.000003    1.651798    0.147956
  O     -0.000000    0.448154   -1.753028

  5
PtN3O- d(N-O)=2.200
  Pt     0.000000   -0.197216    0.177482
  N     -1.468785   -0.963998    0.668197
  N      1.468787   -0.963993    0.668197
  N     -0.000003    1.648944    0.120276
  O     -0.000000    0.476262   -1.741126

  5
PtN3O- d(N-O)=2.150
  Pt     0.000000   -0.211000    0.173050
  N     -1.468380   -0.968305    0.676706
  N      1.468383   -0.968300    0.676706
  N     -0.000003    1.645865    0.093429
  O     -0.000000    0.501740   -1.726866

  5
```

PtN3O- d(N-O)=2.100

Pt	0.000000	-0.223013	0.168779
N	-1.467614	-0.972451	0.684272
N	1.467617	-0.972446	0.684273
N	-0.000003	1.642306	0.067088
O	-0.000000	0.525604	-1.711388

5

PtN3O- d(N-O)=2.050

Pt	0.000000	-0.233648	0.164849
N	-1.466703	-0.976430	0.691014
N	1.466706	-0.976425	0.691015
N	-0.000003	1.638337	0.041122
O	-0.000000	0.548167	-1.694974

5

PtN3O- d(N-O)=2.000

Pt	0.000000	-0.243140	0.161437
N	-1.465735	-0.980313	0.697090
N	1.465738	-0.980308	0.697090
N	-0.000003	1.633969	0.015392
O	-0.000001	0.569792	-1.677985

5

PtN3O- d(N-O)=1.950

Pt	0.000000	-0.251671	0.158635
N	-1.464717	-0.984132	0.702929
N	1.464720	-0.984127	0.702930
N	-0.000002	1.628627	-0.010135
O	-0.000001	0.591303	-1.661334

5

PtN3O- d(N-O)=1.900

Pt	0.000000	-0.259478	0.156322
N	-1.463674	-0.987895	0.708747
N	1.463677	-0.987891	0.708748
N	-0.000002	1.622210	-0.035473
O	-0.000001	0.613054	-1.645319

5

PtN3O- d(N-O)=1.850

Pt	0.000000	-0.266784	0.154372
N	-1.462688	-0.991643	0.714332
N	1.462690	-0.991639	0.714332
N	-0.000002	1.615466	-0.060722
O	-0.000001	0.634600	-1.629289

5

PtN3O- d(N-O)=1.800

Pt	0.000000	-0.273452	0.152847
N	-1.462086	-0.995441	0.719600
N	1.462089	-0.995437	0.719601
N	-0.000002	1.608574	-0.085945
O	-0.000001	0.655756	-1.613079

5

PtN3O- d(N-O)=1.750

Pt	0.000000	-0.280260	0.151308
N	-1.461252	-0.999082	0.725097
N	1.461254	-0.999078	0.725097
N	-0.000002	1.600957	-0.110993
O	-0.000001	0.677463	-1.597485

5

PtN3O- d(N-O)=1.700

Pt	0.000000	-0.286757	0.150146
N	-1.460524	-1.002781	0.730657
N	1.460527	-1.002776	0.730658
N	-0.000002	1.592765	-0.136002
O	-0.000001	0.699548	-1.582433

5

PtN3O- d(N-O)=1.650

Pt	0.000000	-0.293172	0.149530
N	-1.459653	-1.006796	0.736347
N	1.459656	-1.006791	0.736348
N	-0.000002	1.584626	-0.161286
O	-0.000001	0.722132	-1.567914

5

PtN3O- d(N-O)=1.600

Pt	0.000000	-0.299494	0.148902
N	-1.459016	-1.010954	0.742277
N	1.459019	-1.010950	0.742277
N	-0.000002	1.576227	-0.186596
O	-0.000001	0.745171	-1.553836

5

PtN3O- d(N-O)=1.550

Pt	0.000000	-0.305924	0.148582
N	-1.458556	-1.015372	0.748502
N	1.458559	-1.015367	0.748503
N	-0.000002	1.567692	-0.212100
O	-0.000001	0.768971	-1.540462

5

PtN3O- d(N-O)=1.500

Pt	0.000000	-0.312606	0.148578
N	-1.458334	-1.020109	0.755121
N	1.458336	-1.020105	0.755121
N	-0.000002	1.559078	-0.237866
O	-0.000001	0.793741	-1.527928

5

PtN3O- d(N-O)=1.450

Pt	0.000000	-0.319734	0.148878
N	-1.458425	-1.025245	0.762271
N	1.458428	-1.025241	0.762272
N	-0.000002	1.550453	-0.263979
O	-0.000001	0.819768	-1.516416

5

PtN3O- d(N-O)=1.400

Pt	0.000000	-0.327442	0.149368
N	-1.459150	-1.030750	0.770117
N	1.459153	-1.030745	0.770117
N	-0.000002	1.541497	-0.290365
O	-0.000001	0.847441	-1.506213

5

PtN3O- d(N-O)=1.350

Pt	0.000000	-0.336323	0.150337
N	-1.460451	-1.036663	0.778732
N	1.460454	-1.036658	0.778733
N	-0.000002	1.532472	-0.317244
O	-0.000001	0.877172	-1.497533

5

PtN3O- d(N-O)=1.330

Pt	0.072853	-0.117143	-0.000000
N	-0.058885	-1.049643	-1.461368
N	-0.058885	-1.049643	1.461369
N	-0.577766	1.699199	0.000001
O	0.746209	1.824014	-0.000001

5

PtN3O- minimum A d(N-N)=2.867

Pt	-0.000000	0.000050	0.008205
N	-1.433251	-0.827594	0.563299
N	1.433251	-0.827593	0.563299
N	0.000000	1.655137	0.563285
O	-0.000000	0.000001	-1.805065

5

PtN3O- d(N-N)=2.850

Pt	-0.000000	0.002437	0.006094
N	-1.425000	-0.831222	0.566165
N	1.425000	-0.831221	0.566165
N	-0.000000	1.657341	0.561540
O	0.000000	0.002666	-1.806941

5

PtN3O- d(N-N)=2.800

Pt	0.000000	0.009501	-0.000150
N	-1.400000	-0.842247	0.574733
N	1.400000	-0.842247	0.574733

```
  N     -0.000000    1.664453    0.556484
  O     -0.000000    0.010541   -1.812777

  5
PtN3O- d(N-N)=2.750
  Pt     0.000000    0.016610   -0.006364
  N     -1.375000   -0.853124    0.583206
  N      1.375000   -0.853123    0.583206
  N     -0.000000    1.671386    0.551555
  O     -0.000000    0.018252   -1.818580

  5
PtN3O- d(N-N)=2.700
  Pt    -0.000000    0.023705   -0.012479
  N     -1.350000   -0.863922    0.591570
  N      1.350000   -0.863922    0.591570
  N     -0.000000    1.678305    0.546701
  O      0.000000    0.025835   -1.824339

  5
PtN3O- d(N-N)=2.650
  Pt    -0.000000    0.030772   -0.018479
  N     -1.325000   -0.874646    0.599826
  N      1.325000   -0.874645    0.599826
  N     -0.000000    1.685209    0.541895
  O     -0.000000    0.033312   -1.830044

  5
PtN3O- d(N-N)=2.600
  Pt    -0.000000    0.037800   -0.024371
  N     -1.300000   -0.885266    0.607970
  N      1.300000   -0.885265    0.607970
  N     -0.000000    1.692064    0.537158
  O     -0.000000    0.040669   -1.835703

  5
PtN3O- d(N-N)=2.550
  Pt    -0.000000    0.044778   -0.030160
  N     -1.275000   -0.895767    0.616005
  N      1.275000   -0.895767    0.616005
  N     -0.000000    1.698849    0.532496
  O     -0.000000    0.047908   -1.841323

  5
PtN3O- d(N-N)=2.500
  Pt    -0.000000    0.051704   -0.035830
  N     -1.250000   -0.906171    0.623939
  N      1.250000   -0.906171    0.623939
  N     -0.000000    1.705577    0.527867
  O     -0.000000    0.055062   -1.846892

  5
PtN3O- d(N-N)=2.450
  Pt    -0.000000    0.058581   -0.041364
  N     -1.225000   -0.916494    0.631771
  N      1.225000   -0.916494    0.631771
  N     -0.000000    1.712262    0.523244
  O     -0.000000    0.062146   -1.852400

  5
PtN3O- d(N-N)=2.400
  Pt    -0.000068    0.209070   -0.158718
  N     -1.199612   -1.038146    0.729987
  N      1.200387   -1.038371    0.728444
  N      0.000521    1.775063    0.537433
  O     -0.001228    0.092385   -1.944124

  5
PtN3O- TS B" DFT(B3LYP)/ZORA d(N-N)=2.390
  Pt     0.040958    0.140858   -0.091187
  N     -0.815569   -1.150058    0.713126
  N      1.551993   -0.827864    0.664697
  N      0.153827    1.755556    0.508631
  O     -0.031207    0.081511   -1.902246

  5
PtN3O- d(N-N)=2.350
  Pt    -0.000070    0.212923   -0.161569
  N     -1.174610   -1.046803    0.736321
  N      1.175390   -1.047024    0.734804
  N      0.000516    1.780350    0.530540
  O     -0.001226    0.100554   -1.947073

  5
PtN3O- d(N-N)=2.300
  Pt    -0.000072    0.216571   -0.164314
  N     -1.149607   -1.054997    0.742315
  N      1.150393   -1.055215    0.740825
  N      0.000510    1.785300    0.523934
  O     -0.001224    0.108343   -1.949737

  5
PtN3O- d(N-N)=2.250
  Pt    -0.000073    0.220165   -0.166957
  N     -1.124603   -1.063312    0.748416
  N      1.125397   -1.063528    0.746960
  N      0.000505    1.790627    0.517590
  O     -0.001226    0.116048   -1.952985

  5
PtN3O- d(N-N)=2.200
  Pt    -0.000075    0.223467   -0.169425
  N     -1.099599   -1.071197    0.754160
  N      1.100401   -1.071411    0.752740
  N      0.000501    1.795415    0.511011
  O     -0.001228    0.123727   -1.955462

  5
PtN3O- d(N-N)=2.150
  Pt    -0.000075    0.226812   -0.171846
  N     -1.074595   -1.078879    0.759759
  N      1.075404   -1.079090    0.758375
  N      0.000498    1.800229    0.504965
  O     -0.001232    0.130930   -1.958230

  5
PtN3O- d(N-N)=2.100
  Pt    -0.000076    0.230135   -0.174210
  N     -1.049592   -1.086545    0.765356
  N      1.050407   -1.086749    0.764007
  N      0.000495    1.804903    0.498745
  O     -0.001233    0.138256   -1.960874

  5
PtN3O- d(N-N)=2.050
  Pt    -0.000078    0.233422   -0.176507
  N     -1.024590   -1.094211    0.770927
  N      1.025409   -1.094407    0.769607
  N      0.000493    1.809671    0.492578
  O     -0.001234    0.145525   -1.963582

  5
PtN3O- d(N-N)=2.000
  Pt    -0.000082    0.236737   -0.178771
  N     -0.999589   -1.101896    0.776486
  N      1.000411   -1.102083    0.775190
  N      0.000490    1.814466    0.486399
  O     -0.001231    0.152777   -1.966281

  5
PtN3O- d(N-N)=1.950
  Pt    -0.000081    0.240058   -0.180830
  N     -0.974590   -1.109809    0.782017
  N      0.975410   -1.109948    0.780784
  N      0.000507    1.819675    0.480129
  O     -0.001246    0.160026   -1.969078

  5
PtN3O- d(N-N)=1.950
  Pt    -0.000062    0.239970   -0.180797
  N     -0.974564   -1.109717    0.781870
  N      0.975436   -1.109945    0.780787
  N      0.000494    1.819719    0.480146
  O     -0.001304    0.159973   -1.968983
```

```
  5
PtN3O- d(N-N)=1.900
  Pt    -0.000083    0.243343   -0.182815
  N     -0.949580   -1.117722    0.787555
  N      0.950420   -1.117914    0.786323
  N      0.000479    1.825033    0.473831
  O     -0.001237    0.167260   -1.971871

  5
PtN3O- d(N-N)=1.850
  Pt    -0.000082    0.246795   -0.185040
  N     -0.924579   -1.125559    0.793192
  N      0.925421   -1.125730    0.792002
  N      0.000482    1.830050    0.467782
  O     -0.001242    0.174444   -1.974914

  5
PtN3O- d(N-N)=1.700
  Pt    -0.000083    0.250255   -0.187100
  N     -0.899575   -1.133773    0.798999
  N      0.900424   -1.133940    0.797843
  N      0.000478    1.835413    0.461214
  O     -0.001244    0.182045   -1.977933

  5
PtN3O- d(N-N)=1.750
  Pt    -0.000084    0.253844   -0.189148
  N     -0.874572   -1.142268    0.804967
  N      0.875427   -1.142431    0.803843
  N      0.000474    1.841020    0.454453
  O     -0.001245    0.189837   -1.981092

  5
PtN3O- d(N-N)=1.700
  Pt    -0.000085    0.257607   -0.191173
  N     -0.849569   -1.151292    0.811259
  N      0.850431   -1.151453    0.810165
  N      0.000469    1.846839    0.446926
  O     -0.001246    0.198300   -1.984154

  5
PtN3O- d(N-N)=1.650
  Pt    -0.000084    0.261623   -0.193320
  N     -0.824565   -1.160567    0.817703
  N      0.825434   -1.160724    0.816645
  N      0.000465    1.853128    0.439777
  O     -0.001249    0.206542   -1.987782

  5
PtN3O- d(N-N)=1.600
  Pt    -0.000086    0.265937   -0.195526
  N     -0.799562   -1.170421    0.824505
  N      0.800438   -1.170571    0.823478
  N      0.000461    1.859939    0.432347
  O     -0.001251    0.215117   -1.991780

  5
PtN3O- d(N-N)=1.550
  Pt    -0.000089    0.270644   -0.197879
  N     -0.774559   -1.181029    0.831766
  N      0.775441   -1.181173    0.830763
  N      0.000457    1.867444    0.424555
  O     -0.001250    0.224115   -1.996182

  5
PtN3O- d(N-N)=1.500
  Pt    -0.000090    0.275847   -0.200427
  N     -0.749555   -1.192514    0.839562
  N      0.750445   -1.192652    0.838593
  N      0.000453    1.875773    0.416429
  O     -0.001253    0.233547   -2.001135

  5
PtN3O- d(N-N)=1.450
  Pt    -0.000094    0.281740   -0.203068
  N     -0.724550   -1.205231    0.848014
  N      0.725449   -1.205365    0.847073
  N      0.000448    1.885245    0.407607
  O     -0.001253    0.243612   -2.006603

  5
PtN3O- d(N-N)=1.400
  Pt    -0.000087    0.288425   -0.206155
  N     -0.699546   -1.218999    0.857094
  N      0.700454   -1.219129    0.856202
  N      0.000442    1.895846    0.398795
  O     -0.001263    0.253859   -2.012914

  5
PtN3O- d(N-N)=1.350
  Pt    -0.000117    0.296165   -0.209701
  N     -0.674538   -1.234220    0.866998
  N      0.675462   -1.234327    0.866133
  N      0.000451    1.907899    0.389693
  O     -0.001257    0.264484   -2.020100

  5
PtN3O- d(N-N)=1.300
  Pt     0.000258    0.305309   -0.213994
  N     -0.649572   -1.251196    0.878025
  N      0.650428   -1.251554    0.877224
  N      0.000266    1.921731    0.380187
  O     -0.001380    0.275712   -2.028418

  5
PtN3O- d(N-N)=1.250
  Pt    -0.000193    0.316302   -0.219432
  N     -0.624517   -1.270358    0.890275
  N      0.625483   -1.270405    0.889468
  N      0.000473    1.937423    0.370935
  O     -0.001245    0.287040   -2.038223

  5
PtN3O- d(N-N)=1.200
  Pt    -0.000943    0.329518   -0.227645
  N     -0.599426   -1.291597    0.904455
  N      0.600573   -1.291119    0.903701
  N      0.000833    1.954620    0.363100
  O     -0.001037    0.298579   -2.050587

  5
PtN3O- minimum C"  d(N-N)=1.187
  Pt     0.014259    0.176760    0.000058
  N     -1.311219    1.287965    0.004712
  N     -0.151463   -1.805239   -0.593237
  N     -0.147466   -1.805412    0.593964
  O      1.609483    1.062365   -0.005497
```

Appendix S3. Cartesian coordinates [Å] (XYZ format) of DFT(M06-L)/SO-ZORA relaxed surface scans steps for investigated reactions paths. In description of each structure its chemical formula and interatomic distance between dissociating ligands are indicated. For energies of structures see Tables S18-S34.

```
5
OsO4 minimum A d(O-O)=2.776
   Os       -0.000000   -0.000023   -0.000011
   O         0.000000    0.000010    1.699949
   O        -0.000000   -1.602748   -0.566651
   O         1.387990    0.801380   -0.566644
   O        -1.387990    0.801381   -0.566644

  5
OsO4 d(O-O)=2.74
   Os        0.000001   -0.006695    0.004667
   O         0.000009   -0.003774    1.705255
   O        -0.000010   -1.609074   -0.564839
   O         1.370000    0.809777   -0.572536
   O        -1.370000    0.809767   -0.572549

  5
OsO4 d(O-O)=2.69
   Os        0.000006   -0.015627    0.010973
   O         0.004189   -0.009164    1.712007
   O        -0.003688   -1.617183   -0.562206
   O         1.344741    0.819073   -0.583684
   O        -1.345248    0.822901   -0.577091

  5
OsO4 d(O-O)=2.64
   Os        0.000102   -0.024461    0.017285
   O         0.028868   -0.012603    1.718570
   O        -0.023434   -1.625721   -0.557771
   O         1.316996    0.820036   -0.611327
   O        -1.322530    0.842749   -0.566758

  5
OsO4 d(O-O)=2.59
   Os        0.000079   -0.033208    0.023562
   O         0.018563   -0.016407    1.725805
   O        -0.015445   -1.634319   -0.554790
   O         1.293304    0.834519   -0.611295
   O        -1.296501    0.849414   -0.583283

  5
OsO4 d(O-O)=2.54
   Os        0.000094   -0.041842    0.029690
   O         0.018771   -0.021266    1.732776
   O        -0.015279   -1.642399   -0.552764
   O         1.268111    0.845607   -0.618710
   O        -1.271697    0.859900   -0.590994

  5
OsO4 d(O-O)=2.49
   Os       -0.000006   -0.049760    0.035315
   O         0.024472   -0.025603    1.738731
   O        -0.025735   -1.649855   -0.549201
   O         1.245432    0.849042   -0.630262
   O        -1.244164    0.876177   -0.594583

  5
OsO4 d(O-O)=2.44
   Os       -0.000469   -0.057822    0.041166
   O         0.031374   -0.029151    1.744754
   O        -0.043146   -1.657462   -0.544804
   O         1.225675    0.847844   -0.642741
   O        -1.213434    0.896591   -0.598376

  5
OsO4 d(O-O)=2.39
   Os       -0.000477   -0.065656    0.046722
   O         0.031434   -0.033466    1.751080
   O        -0.043260   -1.664938   -0.542688
   O         1.200705    0.857952   -0.649664
   O        -1.188401    0.906108   -0.605451

  5
OsO4 d(O-O)=2.34
   Os       -0.000494   -0.073051    0.051938
   O         0.031732   -0.038581    1.756623
   O        -0.043299   -1.671843   -0.539833
   O         1.175598    0.868434   -0.656003
   O        -1.163537    0.915041   -0.612726

  5
OsO4 d(O-O)=2.29
   Os       -0.000441   -0.080433    0.057171
   O         0.033946   -0.042637    1.762529
   O        -0.044798   -1.678973   -0.537318
   O         1.150182    0.877700   -0.663984
   O        -1.138889    0.924343   -0.618399

  5
OsO4 d(O-O)=2.24
   Os       -0.000846   -0.087362    0.062181
   O         0.059746   -0.048488    1.767081
   O        -0.077496   -1.684707   -0.533210
   O         1.127930    0.871092   -0.687080
   O        -1.109335    0.949465   -0.608972

  5
OsO4 d(O-O)=2.19
   Os       -0.000892   -0.094288    0.067120
   O         0.059985   -0.053089    1.772586
   O        -0.077498   -1.691376   -0.530753
   O         1.102870    0.881254   -0.692728
   O        -1.084465    0.957499   -0.616226

  5
OsO4 d(O-O)=2.14
   Os       -0.000988   -0.100915    0.071810
   O         0.060151   -0.057904    1.777757
   O        -0.077418   -1.697877   -0.527961
   O         1.077824    0.891168   -0.698272
   O        -1.059570    0.965529   -0.623335

  5
OsO4 d(O-O)=2.09
   Os       -0.000544   -0.107492    0.076437
   O         0.037387   -0.061583    1.783875
   O        -0.045562   -1.705362   -0.526570
   O         1.048893    0.916036   -0.689788
   O        -1.040175    0.958402   -0.643955

  5
OsO4 d(O-O)=2.04
   Os       -0.000556   -0.113324    0.080661
   O         0.067371   -0.068278    1.787178
   O        -0.076371   -1.710320   -0.521588
   O         1.023449    0.912463   -0.712964
   O        -1.013893    0.979459   -0.633288

  5
OsO4 d(O-O)=1.99
   Os       -0.000194   -0.119663    0.085096
   O         0.041744   -0.071690    1.793033
   O        -0.044641   -1.717303   -0.520360
   O         0.996068    0.935350   -0.703179
   O        -0.992977    0.973306   -0.654591

  5
OsO4 d(O-O)=1.94
   Os       -0.001421   -0.196466    0.139861
   O         0.071521   -0.086466    1.832480
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```
   O        -0.085005   -1.759041   -0.518770
   O         0.976014    0.985844   -0.766212
   O        -0.961109    1.056128   -0.687359

  5
OsO4 d(O-O)=1.89
   Os       -0.000681   -0.005240    0.017019
   O        -0.321752   -0.860972   -1.508906
   O        -1.358376    0.472957    0.917391
   O         0.328337    0.913283   -1.470173
   O         1.352472   -0.520026    0.903937

  5
OsO4 d(O-O)=1.84
   Os       -0.000684   -0.005287    0.021365
   O        -0.313136   -0.837329   -1.516418
   O        -1.357786    0.472575    0.923284
   O         0.319781    0.889981   -1.478781
   O         1.351826   -0.519938    0.909818

  5
OsO4 d(O-O)=1.79
   Os       -0.000424   -0.004332    0.026732
   O        -0.303699   -0.813916   -1.522572
   O        -1.359066    0.472770    0.928128
   O         0.310531    0.867035   -1.487575
   O         1.352659   -0.521557    0.914555

  5
OsO4 d(O-O)=1.74
   Os       -0.001149   -0.007145    0.106152
   O        -0.387628   -0.752722   -1.606263
   O        -1.295257    0.627873    0.977403
   O         0.392157    0.802464   -1.575739
   O         1.291877   -0.670468    0.957716

  5
OsO4 d(O-O)=1.69
   Os       -0.000691   -0.006835    0.109238
   O        -0.273369   -0.770368   -1.613817
   O        -1.369952    0.449186    0.977872
   O         0.279948    0.826121   -1.579710
   O         1.364063   -0.498103    0.965684

  5
OsO4 d(O-O)=1.64
   Os        0.000143   -0.003606    0.112300
   O        -0.143562   -0.788180   -1.613613
   O        -1.424604    0.238434    0.977900
   O         0.145604    0.825972   -1.591384
   O         1.422419   -0.272619    0.974065

  5
OsO4 d(O-O)=1.59
   Os       -0.000026    0.000135    0.115334
   O         0.000124   -0.794887   -1.608039
   O        -1.445760   -0.000221    0.979897
   O         0.000090    0.795113   -1.608045
   O         1.445574   -0.000140    0.980121

  5
OsO4 d(O-O)=1.54
   Os       -0.000027    0.000042    0.118125
   O        -0.000158   -0.769886   -1.613825
   O        -1.444800    0.000353    0.984248
   O         0.000374    0.770114   -1.613753
   O         1.444611   -0.000624    0.984474

  5
OsO4 d(O-O)=1.49
   Os       -0.000027   -0.000017    0.120808
   O         0.000017   -0.744881   -1.619772
   O        -1.443601    0.000067    0.988838
   O         0.000200    0.745119   -1.619670
   O         1.443411   -0.000288    0.989064

  5
OsO4 d(O-O)=1.44
   Os       -0.000027   -0.000053    0.123033
   O         0.000009   -0.719785   -1.626634
   O        -1.441517    0.000010    0.994529
   O         0.000209    0.720215   -1.626415
   O         1.441327   -0.000386    0.994755

5
OsO4 O-O minimum C d(O-O)=1.428
   Os       -0.000027   -0.000053    0.124077
   O         0.000010   -0.713693   -1.627724
   O        -1.441804    0.000010    0.995098
   O         0.000208    0.714123   -1.627507
   O         1.441613   -0.000386    0.995324

5
OsO3N- minimum A d(O-O)=2.868
   Os        0.000000    0.000047   -0.017347
   O        -1.433949   -0.827983    0.537317
   O         1.433949   -0.827983    0.537317
   O        -0.000001    1.655902    0.537278
   N         0.000000    0.000019   -1.701542

  5
OsO3N- d(O-O)=2.84
   Os       -0.004455   -0.002549   -0.020351
   O        -1.438516   -0.830585    0.535321
   O         1.432923   -0.812370    0.541623
   O         0.012976    1.647173    0.541585
   N        -0.002929   -0.001667   -1.705154

  5
OsO3N- d(O-O)=2.79
   Os       -0.012474   -0.007207   -0.025977
   O        -1.444546   -0.836580    0.534668
   O         1.432424   -0.782158    0.548379
   O         0.034017    1.632082    0.547370
   N        -0.009422   -0.006136   -1.711417

  5
OsO3N- d(O-O)=2.74
   Os       -0.020190   -0.011694   -0.031236
   O        -1.464274   -0.821717    0.529269
   O         1.418831   -0.758114    0.578991
   O         0.064981    1.623611    0.533436
   N         0.000651   -0.032084   -1.717436

  5
OsO3N- d(O-O)=2.69
   Os       -0.028106   -0.016342   -0.036697
   O        -1.466870   -0.831417    0.532427
   O         1.422033   -0.727832    0.576467
   O         0.085775    1.606587    0.544750
   N        -0.012833   -0.030995   -1.723924

  5
OsO3N- d(O-O)=2.64
   Os       -0.035573   -0.020417   -0.041716
   O        -1.473929   -0.836557    0.528622
   O         1.418991   -0.699655    0.584421
   O         0.107179    1.591119    0.551208
   N        -0.016669   -0.034487   -1.729512

  5
OsO3N- d(O-O)=2.59
   Os       -0.042735   -0.025273   -0.046909
   O        -1.482357   -0.839634    0.524554
   O         1.416072   -0.673374    0.591394
   O         0.129634    1.574324    0.559266
   N        -0.020615   -0.036041   -1.735283

  5
OsO3N- d(O-O)=2.54
   Os       -0.050172   -0.028855   -0.051991
   O        -1.488785   -0.845101    0.521464
   O         1.412571   -0.645346    0.598756
   O         0.150806    1.558848    0.566001
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   N        -0.024421   -0.039544   -1.741207

  5
OsO3N- d(O-O)=2.49
   Os       -0.056969   -0.033532   -0.056842
   O        -1.502258   -0.837984    0.518228
   O         1.404568   -0.619116    0.616202
   O         0.176010    1.546013    0.561799
   N        -0.021351   -0.055379   -1.746363

  5
OsO3N- d(O-O)=2.44
   Os       -0.063992   -0.036999   -0.061796
   O        -1.508094   -0.843438    0.515435
   O         1.400813   -0.591326    0.622718
   O         0.196692    1.530177    0.568703
   N        -0.025420   -0.058411   -1.752037

  5
OsO3N- d(O-O)=2.39
   Os       -0.070393   -0.041418   -0.066437
   O        -1.518473   -0.840918    0.512160
   O         1.395094   -0.564929    0.634024
   O         0.219642    1.515060    0.570321
   N        -0.025870   -0.067793   -1.757045

  5
OsO3N- d(O-O)=2.34
   Os       -0.076842   -0.044968   -0.071089
   O        -1.510084   -0.870597    0.509466
   O         1.402199   -0.531648    0.620791
   O         0.228736    1.492704    0.596602
   N        -0.044009   -0.045489   -1.762747

  5
OsO3N- d(O-O)=2.29
   Os       -0.082766   -0.049188   -0.075627
   O        -1.519352   -0.868864    0.506814
   O         1.397822   -0.507539    0.627032
   O         0.252209    1.475155    0.602655
   N        -0.047914   -0.049562   -1.767851

  5
OsO3N- d(O-O)=2.24
   Os       -0.089186   -0.052002   -0.080069
   O        -1.509300   -0.899731    0.504529
   O         1.403489   -0.473572    0.614884
   O         0.261609    1.453490    0.626725
   N        -0.066613   -0.028183   -1.773045

  5
OsO3N- d(O-O)=2.19
   Os       -0.094383   -0.056328   -0.084211
   O        -1.530124   -0.877623    0.501164
   O         1.388985   -0.450815    0.641318
   O         0.290427    1.443497    0.612094
   N        -0.054906   -0.058729   -1.777343

  5
OsO3N- d(O-O)=2.14
   Os       -0.100376   -0.059043   -0.088423
   O        -1.519215   -0.908417    0.500002
   O         1.394417   -0.417271    0.628478
   O         0.300180    1.421805    0.635273
   N        -0.075006   -0.037073   -1.782307

  5
OsO3N- d(O-O)=2.09
   Os       -0.105341   -0.062863   -0.092312
   O        -1.542668   -0.881220    0.496412
   O         1.379460   -0.399222    0.652158
   O         0.332857    1.409610    0.623018
   N        -0.064308   -0.066303   -1.786253

  5
OsO3N- d(O-O)=2.04
   Os       -0.110753   -0.065543   -0.096612
   O        -1.544594   -0.891435    0.492083
   O         1.374782   -0.371404    0.656648
   O         0.349797    1.392228    0.631991
   N        -0.069234   -0.063844   -1.791087

  5
OsO3N- d(O-O)=1.99
   Os       -0.183965   -0.107688   -0.137813
   O        -1.592064   -0.943909    0.475281
   O         1.444801   -0.308292    0.679004
   O         0.433475    1.405518    0.692303
   N        -0.102249   -0.045627   -1.815752

  5
OsO3N- d(O-O)=1.94
   Os       -0.187737   -0.109979   -0.139515
   O        -1.601304   -0.937930    0.473494
   O         1.434504   -0.283606    0.689093
   O         0.454470    1.390650    0.687556
   N        -0.099934   -0.059133   -1.817605

  5
OsO3N- d(O-O)=1.89
   Os       -0.190878   -0.111773   -0.142541
   O        -1.603309   -0.942171    0.470704
   O         1.427893   -0.258389    0.692193
   O         0.471349    1.371678    0.693979
   N        -0.105056   -0.059343   -1.821312

  5
OsO3N- d(O-O)=1.84
   Os       -0.194125   -0.113840   -0.144669
   O        -1.607072   -0.944619    0.467777
   O         1.421000   -0.233390    0.694443
   O         0.488309    1.352697    0.698417
   N        -0.108112   -0.060846   -1.822946

  5
OsO3N- d(O-O)=1.79
   Os       -0.197469   -0.115767   -0.147187
   O        -1.624667   -0.923494    0.464875
   O         1.405230   -0.211205    0.714475
   O         0.513209    1.340446    0.686606
   N        -0.096305   -0.089977   -1.825746

  5
OsO3N- d(O-O)=1.74
   Os       -0.012033    0.126474   -0.003001
   O        -0.955823    1.275616    0.900928
   O        -0.650328   -1.673016   -0.500421
   O         0.593512   -1.607525    0.714557
   N         1.038263    0.794889   -1.112062

  5
OsO3N- d(O-O)=1.69
   Os       -0.012236    0.129479   -0.002535
   O        -1.066261    1.274087    0.776829
   O        -0.562406   -1.673478   -0.570547
   O         0.481541   -1.618626    0.757333
   N         1.172953    0.804975   -0.961078

  5
OsO3N- d(O-O)=1.64
   Os       -0.011132    0.132115    0.000367
   O        -1.171427    1.272947    0.618420
   O        -0.455036   -1.670514   -0.642741
   O         0.346653   -1.633391    0.787475
   N         1.304533    0.815281   -0.763519

  5
OsO3N- d(O-O)=1.59
   Os       -0.011261    0.135422    0.002182
   O        -1.254196    1.272856    0.439601
   O        -0.338844   -1.665652   -0.699714
   O         0.207988   -1.648386    0.793195
   N         1.409904    0.822198   -0.535262
```

```
  5
OsO3N- d(O-O)=1.54
   Os       -0.011726    0.138307    0.002537
   O        -1.310997    1.273626    0.235387
   O        -0.211716   -1.664190   -0.735720
   O         0.067782   -1.658517    0.778694
   N         1.480247    0.827213   -0.280896

  5
OsO3N- d(O-O)=1.49
   Os       -0.012610    0.141380    0.000064
   O        -1.332685    1.276948    0.004426
   O        -0.076050   -1.665579   -0.744812
   O        -0.071121   -1.665613    0.745180
   N         1.506056    0.829302   -0.004856

  5
OsO3N- d(O-O)=1.44
   Os       -0.012931    0.144460    0.000111
   O        -1.332618    1.280907    0.004771
   O        -0.075885   -1.670280   -0.719880
   O        -0.070845   -1.670453    0.720112
   N         1.505870    0.831804   -0.005113

5
OsO3N- minimum C d(O-O)=1.45
   Os        -0.013019   0.143832   0.000116
   O         -1.332446   1.280581   0.004769
   O         -0.075833  -1.669624  -0.723608
   O         -0.070768  -1.669801   0.723839
   N          1.505657   0.831450  -0.005114

5
OsO3N- minimum A d(N-O)=2.785
   Os         0.000000   0.000047  -0.017347
   O         -1.433949  -0.827983   0.537317
   O          1.433949  -0.827983   0.537317
   O         -0.000001   1.655902   0.537278
   N          0.000000   0.000019  -1.701542

  5
OsO3N- d(N-O)=2.77
   Os        0.000005   -0.002189   -0.015264
   O        -1.434783   -0.830048    0.538445
   O         1.434786   -0.830060    0.538443
   O        -0.000010    1.654864    0.529127
   N        -0.000000    0.007436   -1.697727

  5
OsO3N- d(N-O)=2.72
   Os       -0.000018   -0.009633   -0.008206
   O        -1.437518   -0.832681    0.548592
   O         1.437324   -0.829167    0.554165
   O        -0.003007    1.656897    0.483345
   N         0.003218    0.014585   -1.684874

  5
OsO3N- d(N-O)=2.67
   Os       -0.000012   -0.017169   -0.001522
   O        -1.439699   -0.838653    0.554917
   O         1.440606   -0.833967    0.559413
   O        -0.003469    1.653734    0.452179
   N         0.002573    0.036057   -1.671964

  5
OsO3N- d(N-O)=2.62
   Os        0.000016   -0.024698    0.005394
   O        -1.441738   -0.846343    0.559353
   O         1.444083   -0.839881    0.562863
   O        -0.004241    1.649688    0.424482
   N         0.001878    0.061237   -1.659069

  5
OsO3N- d(N-O)=2.57
   Os       -0.000107   -0.032035    0.012431
   O        -1.444095   -0.862276    0.550427
   O         1.447197   -0.835395    0.581437
   O        -0.019650    1.646028    0.394492
   N         0.016654    0.083680   -1.645765

  5
OsO3N- d(N-O)=2.52
   Os        0.000123   -0.039626    0.018334
   O        -1.445986   -0.869315    0.554339
   O         1.450107   -0.841587    0.585198
   O        -0.020315    1.641281    0.367820
   N         0.016069    0.109249   -1.632668

  5
OsO3N- d(N-O)=2.47
   Os       -0.000257   -0.047324    0.024642
   O        -1.448944   -0.885693    0.542892
   O         1.452583   -0.843272    0.595397
   O        -0.030302    1.634812    0.348355
   N         0.026918    0.141479   -1.618262

  5
OsO3N- d(N-O)=2.42
   Os        0.000149   -0.054634    0.030582
   O        -1.451125   -0.892021    0.545567
   O         1.454791   -0.850777    0.598714
   O        -0.030215    1.630127    0.322583
   N         0.026398    0.167307   -1.604423

  5
OsO3N- d(N-O)=2.37
   Os       -0.000245   -0.062892    0.035755
   O        -1.454526   -0.902012    0.542590
   O         1.457212   -0.857926    0.601041
   O        -0.030939    1.623678    0.303404
   N         0.028497    0.199154   -1.589768

  5
OsO3N- d(N-O)=2.32
   Os       -0.000436   -0.070366    0.041092
   O        -1.454996   -0.924669    0.522860
   O         1.458847   -0.848147    0.627077
   O        -0.053174    1.618555    0.276845
   N         0.049757    0.224629   -1.574851

  5
OsO3N- d(N-O)=2.27
   Os       -0.000638   -0.079341    0.044966
   O        -1.455517   -0.949111    0.500649
   O         1.461144   -0.841695    0.647182
   O        -0.072875    1.611244    0.258995
   N         0.067885    0.258905   -1.558769

  5
OsO3N- d(N-O)=2.22
   Os       -0.000533   -0.087339    0.049708
   O        -1.455256   -0.968250    0.485367
   O         1.461807   -0.831043    0.674791
   O        -0.091768    1.606846    0.226988
   N         0.085748    0.279788   -1.543832

  5
OsO3N- d(N-O)=2.17
   Os       -0.000425   -0.096885    0.053190
   O        -1.454509   -0.988655    0.471503
   O         1.463190   -0.818168    0.702658
   O        -0.110263    1.601639    0.195241
   N         0.102007    0.302072   -1.529569

  5
OsO3N- d(N-O)=2.12
   Os       -0.000018   -0.106977    0.057162
   O        -1.454292   -1.006271    0.458264
   O         1.461924   -0.803952    0.736393
   O        -0.128163    1.598209    0.156687
   N         0.120549    0.318993   -1.515482

  5
OsO3N- d(N-O)=2.07
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```
   Os        0.000789   -0.121382    0.057924
   O        -1.461197   -0.994086    0.488427
   O         1.467748   -0.828742    0.715288
   O        -0.102102    1.596807    0.135012
   N         0.094762    0.347405   -1.503628

  5
OsO3N- d(N-O)=2.02
   Os        0.002997   -0.147718    0.055528
   O        -1.461071   -1.021394    0.469481
   O         1.467967   -0.814999    0.752624
   O        -0.125534    1.601018    0.104390
   N         0.115640    0.383095   -1.489002

5
OsO3N- TS B' d(N-O)=1.977
   Os        0.000351   -0.223487    0.101351
   O        -1.481797   -0.965848    0.625326
   O         1.486187   -0.971796    0.606067
   O         0.003835    1.713199    0.039719
   N        -0.008578    0.447932   -1.479439

  5
OsO3N- d(N-O)=1.97
   Os        0.003404   -0.224017    0.106679
   O        -1.467386   -1.072240    0.477659
   O         1.479649   -0.864467    0.763032
   O        -0.124772    1.711450    0.020008
   N         0.109103    0.449276   -1.474354

  5
OsO3N- d(N-O)=1.92
   Os        0.001521   -0.230411    0.130749
   O        -1.466143   -1.087076    0.478229
   O         1.480422   -0.879355    0.763520
   O        -0.121970    1.718741   -0.016002
   N         0.106169    0.478103   -1.463473

  5
OsO3N- d(N-O)=1.87
   Os        0.000078   -0.233359    0.148289
   O        -1.463919   -1.097767    0.480331
   O         1.479363   -0.890395    0.765445
   O        -0.118870    1.715338   -0.045989
   N         0.103348    0.506184   -1.455054

  5
OsO3N- d(N-O)=1.82
   Os       -0.001302   -0.234976    0.162575
   O        -1.461878   -1.106034    0.482919
   O         1.477931   -0.898540    0.767701
   O        -0.115386    1.705896   -0.072411
   N         0.100634    0.533656   -1.447761

  5
OsO3N- d(N-O)=1.77
   Os       -0.002289   -0.235281    0.174265
   O        -1.459348   -1.112953    0.485711
   O         1.475999   -0.906064    0.770209
   O        -0.112297    1.694183   -0.097276
   N         0.097934    0.560117   -1.439885

  5
OsO3N- d(N-O)=1.72
   Os       -0.002992   -0.235389    0.184388
   O        -1.457744   -1.118606    0.487857
   O         1.475044   -0.912521    0.772351
   O        -0.109411    1.681960   -0.121515
   N         0.095102    0.584559   -1.430059

  5
OsO3N- d(N-O)=1.67
   Os       -0.004056   -0.234887    0.192269
   O        -1.454604   -1.125472    0.491207
   O         1.472087   -0.919157    0.774914
   O        -0.105854    1.670017   -0.145327
   N         0.092426    0.609502   -1.420040

  5
OsO3N- d(N-O)=1.62
   Os       -0.004849   -0.235139    0.200112
   O        -1.453223   -1.131462    0.492979
   O         1.471195   -0.925178    0.776420
   O        -0.102705    1.660085   -0.169810
   N         0.089580    0.631696   -1.406678

  5
OsO3N- d(N-O)=1.57
   Os       -0.005471   -0.234920    0.206064
   O        -1.450250   -1.138272    0.496327
   O         1.468598   -0.932328    0.779192
   O        -0.099624    1.650114   -0.194129
   N         0.086746    0.655407   -1.394431

  5
OsO3N- d(N-O)=1.52
   Os       -0.006055   -0.235078    0.211963
   O        -1.448275   -1.144194    0.498420
   O         1.467086   -0.938441    0.780931
   O        -0.096576    1.640766   -0.218432
   N         0.083818    0.676949   -1.379859

  5
OsO3N- d(N-O)=1.47
   Os       -0.006443   -0.235574    0.216129
   O        -1.445364   -1.151170    0.502175
   O         1.464494   -0.945756    0.784136
   O        -0.093561    1.632239   -0.243039
   N         0.080873    0.700262   -1.366379

  5
OsO3N- d(N-O)=1.42
   Os       -0.006950   -0.235866    0.221571
   O        -1.443024   -1.158026    0.504692
   O         1.462690   -0.952903    0.786243
   O        -0.090601    1.624933   -0.268336
   N         0.077885    0.721864   -1.351147

5
OsO3N- minimum C' d(N-O)=1.402
   Os       -0.058118   -0.068631    0.000000
   O         0.022235   -0.990204   -1.461533
   O         0.022237   -0.990204    1.461533
   O        -0.626151    1.772898    0.000000
   N         0.763324    1.582924   -0.000000

5
IrO4+ minimum A d(O-O)=2.759
   Ir        0.000000    0.000027   -0.021381
   O        -1.379634   -0.796559    0.541834
   O         1.379632   -0.796559    0.541840
   O        -0.000001    1.593104    0.541841
   O         0.000004   -0.000013   -1.711110

  5
IrO4+ d(O-O)=2.72
   Ir        0.000001   -0.007367   -0.016137
   O        -1.381338   -0.802156    0.545795
   O         1.381337   -0.802171    0.545781
   O        -0.000014    1.591065    0.519213
   O         0.000016    0.020630   -1.701628

  5
IrO4+ d(O-O)=2.67
   Ir       -0.000000   -0.016252   -0.009903
   O        -1.382932   -0.810117    0.549578
   O         1.382875   -0.810901    0.548601
   O         0.000631    1.587089    0.494025
   O        -0.000572    0.050180   -1.689277

  5
IrO4+ d(O-O)=2.62
   Ir        0.000006   -0.025131   -0.003416
   O        -1.385200   -0.799110    0.578553
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```
   O         1.384572   -0.827018    0.541181
   O         0.022335    1.587394    0.453872
   O        -0.021712    0.063865   -1.677166

  5
IrO4+ d(O-O)=2.57
   Ir       -0.000006   -0.033728    0.002657
   O        -1.387715   -0.803645    0.584091
   O         1.384491   -0.838052    0.543334
   O         0.026485    1.583377    0.427698
   O        -0.023254    0.092049   -1.664756

  5
IrO4+ d(O-O)=2.52
   Ir       -0.000161   -0.042241    0.008648
   O        -1.390707   -0.809382    0.587861
   O         1.386010   -0.845618    0.548131
   O         0.026151    1.579396    0.400352
   O        -0.021292    0.117845   -1.651968

  5
IrO4+ d(O-O)=2.47
   Ir       -0.000082   -0.050188    0.014531
   O        -1.391636   -0.824588    0.581930
   O         1.387621   -0.841632    0.567326
   O         0.012330    1.576740    0.369021
   O        -0.008232    0.139667   -1.639784

  5
IrO4+ d(O-O)=2.42
   Ir       -0.000314   -0.058307    0.020185
   O        -1.395394   -0.821300    0.595212
   O         1.387520   -0.859393    0.560003
   O         0.025598    1.571680    0.343992
   O        -0.017409    0.167320   -1.626369

  5
IrO4+ d(O-O)=2.37
   Ir       -0.000292   -0.065693    0.025533
   O        -1.396250   -0.833349    0.592715
   O         1.388424   -0.860089    0.573201
   O         0.017989    1.567928    0.315250
   O        -0.009870    0.191202   -1.613675

  5
IrO4+ d(O-O)=2.32
   Ir       -0.000330   -0.073287    0.030946
   O        -1.398039   -0.838429    0.598308
   O         1.390155   -0.866907    0.576362
   O         0.017377    1.563254    0.287752
   O        -0.009162    0.215369   -1.600343

  5
IrO4+ d(O-O)=2.27
   Ir       -0.000350   -0.080230    0.036148
   O        -1.398657   -0.861588    0.579891
   O         1.390770   -0.853227    0.609416
   O        -0.006512    1.559767    0.255491
   O         0.014749    0.235277   -1.587923

  5
IrO4+ d(O-O)=2.22
   Ir       -0.000432   -0.087402    0.040913
   O        -1.399329   -0.883905    0.561585
   O         1.391658   -0.848224    0.629049
   O        -0.026203    1.553465    0.234528
   O         0.034307    0.266065   -1.573051

  5
IrO4+ d(O-O)=2.17
   Ir       -0.000385   -0.093610    0.045621
   O        -1.398412   -0.905025    0.546087
   O         1.390400   -0.835978    0.660106
   O        -0.046538    1.549142    0.201193
   O         0.054936    0.285470   -1.559982

  5
IrO4+ d(O-O)=2.12
   Ir       -0.000748   -0.183373    0.109057
   O        -1.442317   -0.943430    0.535165
   O         1.434764   -0.842786    0.693731
   O        -0.066067    1.598313    0.139083
   O         0.074369    0.371276   -1.584012

  5
IrO4+ d(O-O)=2.07
   Ir       -0.000641   -0.187070    0.111355
   O        -1.437782   -0.964625    0.520363
   O         1.431389   -0.836377    0.715465
   O        -0.080141    1.591390    0.113989
   O         0.087176    0.396683   -1.568147

  5
IrO4+ d(O-O)=2.07
   Ir       -0.011971    0.035733   -0.001923
   O        -1.139227   -0.661149   -1.041620
   O         0.833218   -0.999453    1.023455
   O        -0.513729    1.579264    0.730389
   O         0.955233    1.352390   -0.710298

  5
IrO4+ d(O-O)=2.02
   Ir       -0.012873    0.030023   -0.002015
   O        -1.140272   -0.666581   -1.041841
   O         0.832441   -1.004908    1.023624
   O        -0.494590    1.584782    0.713104
   O         0.938818    1.363468   -0.692869

  5
IrO4+ d(O-O)=1.97
   Ir       -0.013234    0.027386   -0.002082
   O        -1.138956   -0.676694   -1.038735
   O         0.828309   -1.014166    1.019996
   O        -0.475149    1.592787    0.696153
   O         0.922554    1.377471   -0.675331

  5
IrO4+ d(O-O)=1.92
   Ir       -0.014083    0.022475   -0.002008
   O        -1.139608   -0.682531   -1.038517
   O         0.827156   -1.019960    1.019592
   O        -0.456111    1.598392    0.678767
   O         0.906170    1.388408   -0.657833

  5
IrO4+ d(O-O)=1.87
   Ir       -0.015953    0.017486   -0.000874
   O        -1.130541   -0.692639   -1.045654
   O         0.806147   -1.023139    1.038074
   O        -0.438728    1.612234    0.646414
   O         0.902599    1.392844   -0.637957

  5
IrO4+ d(O-O)=1.82
   Ir       -0.031364   -0.060600    0.000741
   O        -1.036064   -0.735677   -1.153584
   O         0.675200   -1.027021    1.168781
   O        -0.460134    1.696125    0.535520
   O         0.975886    1.433959   -0.551456

  5
IrO4+ d(O-O)=1.77
   Ir       -0.030174   -0.063625   -0.000374
   O        -0.917828   -0.763494   -1.232888
   O         0.569877   -1.014526    1.237667
   O        -0.494037    1.702754    0.458106
   O         0.995687    1.445676   -0.462509

  5
IrO4+ d(O-O)=1.72
   Ir       -0.029406   -0.067389   -0.000697
   O        -0.741928   -0.798450   -1.325002
   O         0.407088   -0.992439    1.322075
   O        -0.532844    1.710612    0.348061
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   O         1.020614    1.454451   -0.344435

  5
IrO4+ d(O-O)=1.67
   Ir       -0.029737   -0.070460   -0.000463
   O        -0.539785   -0.838181   -1.395442
   O         0.200974   -0.965014    1.393092
   O        -0.549246    1.722036    0.219067
   O         1.041318    1.458404   -0.216252

  5
IrO4+ d(O-O)=1.62
   Ir       -0.030577   -0.072446   -0.000212
   O        -0.539994   -0.844850   -1.392440
   O         0.199440   -0.971592    1.390014
   O        -0.524125    1.725837    0.212452
   O         1.018780    1.469836   -0.209813

  5
IrO4+ d(O-O)=1.57
   Ir       -0.033934   -0.075406    0.000290
   O        -0.431062   -0.869922   -1.416156
   O         0.080311   -0.958062    1.415575
   O        -0.507036    1.735467    0.141184
   O         1.015245    1.474708   -0.140890

  5
IrO4+ d(O-O)=1.52
   Ir       -0.033779   -0.078174   -0.000004
   O        -0.178398   -0.920491   -1.436500
   O        -0.178704   -0.920453    1.436481
   O        -0.491798    1.741784   -0.000852
   O         1.006203    1.484119    0.000877

  5
IrO4+ d(O-O)=1.47
   Ir       -0.034385   -0.080762    0.000001
   O        -0.179522   -0.928279   -1.433742
   O        -0.179955   -0.928219    1.433736
   O        -0.465606    1.746989   -0.000109
   O         0.982992    1.497057    0.000116

  5
IrO4+ d(O-O)=1.42
   Ir        0.012366   -0.088871    0.000000
   O        -0.017853   -0.952360   -1.431314
   O        -0.017853   -0.952359    1.431315
   O        -0.636135    1.674976    0.000000
   O         0.782999    1.625399    0.000000

5
IrO4+ minimum C d(O-O)=1.385
   Ir        0.012407   -0.091246    0.000001
   O        -0.018103   -0.958365   -1.429211
   O        -0.018103   -0.958365    1.429212
   O        -0.618602    1.681572    0.000000
   O         0.765925    1.633189   -0.000000

5
IrNO3 minimum A d(O-O)=2.836
   Ir        0.000000    0.000035  -0.011190
   O        -1.418238   -0.818843   0.529997
   O         1.418239   -0.818844   0.529995
   O        -0.000000    1.637678   0.530019
   N         0.000001   -0.000024  -1.685800

  5
IrNO3 d(O-O)=2.82
   Ir       -0.002774   -0.001552   -0.013491
   O        -1.420364   -0.820111    0.529853
   O         1.417007   -0.810005    0.532382
   O         0.007074    1.632226    0.532385
   N        -0.000942   -0.000556   -1.688108

  5
IrNO3 d(O-O)=2.77
   Ir       -0.011119   -0.006370   -0.018381
   O        -1.426448   -0.824238    0.532059
   O         1.418907   -0.782306    0.532667
   O         0.035392    1.617430    0.539999
   N        -0.016729   -0.004515   -1.693323

  5
IrNO3 d(O-O)=2.72
   Ir       -0.019314   -0.010968   -0.023714
   O        -1.445130   -0.809589    0.528094
   O         1.406860   -0.757569    0.561849
   O         0.067047    1.609282    0.525506
   N        -0.009462   -0.031154   -1.698715

  5
IrNO3 d(O-O)=2.67
   Ir       -0.027231   -0.015534   -0.029128
   O        -1.462014   -0.800170    0.520169
   O         1.395881   -0.728615    0.592111
   O         0.092158    1.600142    0.514028
   N         0.001208   -0.055821   -1.704159

  5
IrNO3 d(O-O)=2.62
   Ir       -0.035087   -0.020308   -0.033814
   O        -1.459766   -0.814374    0.528330
   O         1.404047   -0.692769    0.585076
   O         0.110053    1.584533    0.522830
   N        -0.019245   -0.057081   -1.709401

  5
IrNO3 d(O-O)=2.57
   Ir       -0.042625   -0.024610   -0.039235
   O        -1.465903   -0.825243    0.517702
   O         1.402634   -0.669425    0.585077
   O         0.131238    1.563702    0.545094
   N        -0.025341   -0.044421   -1.715616

  5
IrNO3 d(O-O)=2.52
   Ir       -0.050159   -0.028586   -0.043930
   O        -1.470404   -0.834219    0.514014
   O         1.403777   -0.647481    0.577512
   O         0.156953    1.542427    0.566010
   N        -0.040164   -0.032139   -1.720584

  5
IrNO3 d(O-O)=2.47
   Ir       -0.057363   -0.032664   -0.049041
   O        -1.478874   -0.835172    0.510678
   O         1.399116   -0.619893    0.589068
   O         0.179738    1.528035    0.568490
   N        -0.042616   -0.040303   -1.726174

  5
IrNO3 d(O-O)=2.42
   Ir       -0.064014   -0.037293   -0.053380
   O        -1.496979   -0.819747    0.505947
   O         1.387254   -0.590917    0.618633
   O         0.205683    1.519972    0.552006
   N        -0.031943   -0.072012   -1.730185

  5
IrNO3 d(O-O)=2.37
   Ir       -0.071057   -0.041116   -0.058634
   O        -1.503489   -0.823610    0.503017
   O         1.383822   -0.564082    0.625051
   O         0.227406    1.503606    0.559719
   N        -0.036681   -0.074797   -1.736131

  5
IrNO3 d(O-O)=2.32
   Ir       -0.077151   -0.044742   -0.062926
   O        -1.508999   -0.828642    0.498212
   O         1.381135   -0.536940    0.629849
   O         0.247783    1.486458    0.568400
   N        -0.042766   -0.076132   -1.740514
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  5
IrNO3 d(O-O)=2.27
   Ir       -0.083980   -0.047656   -0.067298
   O        -1.503849   -0.853216    0.494306
   O         1.387119   -0.510307    0.614810
   O         0.264533    1.462604    0.596909
   N        -0.063821   -0.051422   -1.745707

  5
IrNO3 d(O-O)=2.22
   Ir       -0.089718   -0.051300   -0.071905
   O        -1.500560   -0.872097    0.490845
   O         1.391812   -0.484118    0.602681
   O         0.281259    1.438041    0.622068
   N        -0.082792   -0.030524   -1.750667

  5
IrNO3 d(O-O)=2.17
   Ir       -0.095301   -0.055013   -0.075884
   O        -1.517628   -0.856622    0.486061
   O         1.379637   -0.457722    0.628025
   O         0.307189    1.428654    0.609613
   N        -0.073895   -0.059295   -1.754793

  5
IrNO3 d(O-O)=2.12
   Ir       -0.101045   -0.057648   -0.080972
   O        -1.523273   -0.861632    0.478581
   O         1.372932   -0.431925    0.637829
   O         0.326231    1.411555    0.617848
   N        -0.074843   -0.060349   -1.760265

  5
IrNO3 d(O-O)=2.07
   Ir       -0.178290   -0.101964   -0.122692
   O        -1.577440   -0.913050    0.474142
   O         1.440824   -0.370047    0.656286
   O         0.407189    1.423351    0.671175
   N        -0.092282   -0.038288   -1.785891

  5
IrNO3 d(O-O)=2.02
   Ir       -0.182245   -0.104180   -0.124876
   O        -1.584966   -0.910054    0.470665
   O         1.431561   -0.345002    0.666473
   O         0.427558    1.407817    0.669109
   N        -0.091907   -0.048579   -1.788350

  5
IrNO3 d(O-O)=1.97
   Ir       -0.185190   -0.105766   -0.127331
   O        -1.587275   -0.916252    0.463153
   O         1.427184   -0.320250    0.668388
   O         0.445144    1.387487    0.679817
   N        -0.099861   -0.045216   -1.791007

  5
IrNO3 d(O-O)=1.92
   Ir       -0.188663   -0.107893   -0.130223
   O        -1.590659   -0.919559    0.458851
   O         1.420433   -0.294884    0.672924
   O         0.462010    1.368748    0.685371
   N        -0.103119   -0.046410   -1.793902

  5
IrNO3 d(O-O)=1.87
   Ir       -0.191822   -0.109486   -0.132560
   O        -1.593829   -0.923340    0.453532
   O         1.415441   -0.269418    0.676883
   O         0.481369    1.350519    0.691487
   N        -0.111158   -0.048272   -1.796321

 5
IrNO3 d(O-O)=1.82
Ir       -0.252311   -0.143702   -0.162635
O        -1.635668   -0.969660    0.433848
O         1.473455   -0.212165    0.694167
O         0.555112    1.358572    0.736948
N        -0.140586   -0.033044   -1.809308

  5
IrNO3 d(O-O)=1.77
   Ir       -0.016777    0.110743   -0.028867
   O        -1.304566    1.205066   -0.335379
   O         0.081777   -1.669404   -0.775590
   O        -0.217826   -1.532628    0.963499
   N         1.470984    0.802660    0.176340

  5
IrNO3 d(O-O)=1.72
   Ir       -0.016832    0.114487   -0.029315
   O        -1.318019    1.218983   -0.220337
   O        -0.004225   -1.676937   -0.745296
   O        -0.136270   -1.534626    0.963713
   N         1.488937    0.794530    0.031237

  5
IrNO3 d(O-O)=1.67
   Ir       -0.017889    0.118180   -0.023794
   O        -1.320400    1.236359   -0.076336
   O        -0.088796   -1.673121   -0.729169
   O        -0.051118   -1.552086    0.936013
   N         1.491794    0.787105   -0.106712

  5
IrNO3 d(O-O)=1.62
   Ir       -0.018040    0.119269   -0.045371
   O        -1.314707    1.224104   -0.265895
   O        -0.024338   -1.717125   -0.624453
   O        -0.119663   -1.505242    0.978799
   N         1.490340    0.795431   -0.043078

  5
IrNO3 d(O-O)=1.57
   Ir       -0.019115    0.126410    0.001263
   O        -1.319477    1.248202    0.004004
   O        -0.071434   -1.628188   -0.784856
   O        -0.066920   -1.629298    0.785137
   N         1.490538    0.799311   -0.005546

  5
IrNO3 d(O-O)=1.52
   Ir       -0.019649    0.129849    0.001347
   O        -1.318646    1.253542    0.003445
   O        -0.070997   -1.634545   -0.759909
   O        -0.066819   -1.635560    0.760085
   N         1.489703    0.803150   -0.004965

  5
IrNO3 d(O-O)=1.47
   Ir       -0.020159    0.133390    0.000440
   O        -1.317514    1.258995    0.004239
   O        -0.071068   -1.641439   -0.734847
   O        -0.066285   -1.641740    0.735146
   N         1.488618    0.807231   -0.004975

  5
IrNO3 d(O-O)=1.42
   Ir       -0.020506    0.136946    0.000137
   O        -1.316397    1.265392    0.004713
   O        -0.071049   -1.649054   -0.709894
   O        -0.066081   -1.649225    0.710097
   N         1.487625    0.812378   -0.005051
5
IrNO3 minimum C d(O-O)=1.414
   Ir       -0.020427    0.137447    0.000135
   O        -1.316534    1.265645    0.004714
   O        -0.071096   -1.649579   -0.706885
   O        -0.066148   -1.649748    0.707088
   N         1.487797    0.812672   -0.005050

5
IrNO3 minimum A d(N-O)=2.755
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   Ir        0.000000   0.000035  -0.011190
   O        -1.418238  -0.818843   0.529997
   O         1.418239  -0.818844   0.529995
   O        -0.000000   1.637678   0.530019
   N         0.000001  -0.000024  -1.685800

  5
IrNO3 d(N-O)=2.75
   Ir        0.000001   -0.000927   -0.010435
   O        -1.418583   -0.819445    0.530372
   O         1.418584   -0.819453    0.530363
   O        -0.000006    1.637191    0.527110
   N         0.000005    0.002635   -1.684389

  5
IrNO3 d(N-O)=2.70
   Ir       -0.000011   -0.008818   -0.003619
   O        -1.419882   -0.837802    0.518395
   O         1.419964   -0.835885    0.521150
   O        -0.001634    1.624896    0.527821
   N         0.001566    0.057611   -1.670726

  5
IrNO3 d(N-O)=2.65
   Ir       -0.000012   -0.017103    0.002982
   O        -1.422275   -0.848443    0.515583
   O         1.421708   -0.847044    0.519351
   O        -0.001555    1.618115    0.511644
   N         0.002136    0.094477   -1.656538

  5
IrNO3 d(N-O)=2.60
   Ir       -0.000014   -0.024843    0.009331
   O        -1.422408   -0.857528    0.520624
   O         1.424177   -0.853207    0.522631
   O        -0.002747    1.615817    0.483444
   N         0.000994    0.119762   -1.643009

  5
IrNO3 d(N-O)=2.55
   Ir       -0.000115   -0.033260    0.015485
   O        -1.425482   -0.871783    0.509610
   O         1.425446   -0.861555    0.526091
   O        -0.008545    1.608588    0.469492
   N         0.008698    0.158013   -1.627657

  5
IrNO3 d(N-O)=2.50
   Ir       -0.000158   -0.041244    0.020781
   O        -1.426920   -0.885562    0.501848
   O         1.425718   -0.875202    0.522044
   O        -0.009230    1.600961    0.459772
   N         0.010592    0.201048   -1.611423

  5
IrNO3 d(N-O)=2.45
   Ir       -0.000317   -0.050306    0.025802
   O        -1.430530   -0.897459    0.492644
   O         1.426895   -0.886910    0.520076
   O        -0.010305    1.593093    0.448929
   N         0.014260    0.241584   -1.594431

  5
IrNO3 d(N-O)=2.40
   Ir       -0.000234   -0.057828    0.031408
   O        -1.431552   -0.897476    0.508926
   O         1.428213   -0.896818    0.518646
   O        -0.001604    1.592889    0.414683
   N         0.005179    0.259235   -1.580641

  5
IrNO3 d(N-O)=2.35
   Ir       -0.000027   -0.066677    0.035856
   O        -1.433778   -0.900898    0.517031
   O         1.430252   -0.907468    0.515761
   O         0.003406    1.589249    0.389876
   N         0.000150    0.285797   -1.565502

  5
IrNO3 d(N-O)=2.30
   Ir       -0.000092   -0.074993    0.040442
   O        -1.434845   -0.909497    0.518277
   O         1.431560   -0.912764    0.521974
   O         0.000992    1.586852    0.362808
   N         0.002387    0.310404   -1.550481

  5
IrNO3 d(N-O)=2.25
   Ir       -0.000200   -0.084285    0.044061
   O        -1.436031   -0.917604    0.521497
   O         1.433669   -0.918553    0.525607
   O         0.000221    1.583897    0.337226
   N         0.002343    0.336547   -1.535370

  5
IrNO3 d(N-O)=2.20
   Ir        0.000393   -0.094146    0.047312
   O        -1.437878   -0.904572    0.556005
   O         1.434718   -0.940602    0.506252
   O         0.023682    1.582614    0.304848
   N        -0.020913    0.356709   -1.521396

  5
IrNO3 d(N-O)=2.15
   Ir       -0.000005   -0.108291    0.051527
   O        -1.441113   -0.914432    0.557495
   O         1.437689   -0.946203    0.513661
   O         0.021522    1.582120    0.278500
   N        -0.018091    0.386808   -1.508162

5
IrNO3 TS B' d(N-O)=2.109
 Ir        0.000000  -0.200517 0.075141
 O        -1.464349 -0.926465 0.602334
 O         1.464350  -0.926472 0.602323
 O        -0.000005 1.678156  0.135885
 N         0.000004  0.375298  -1.522659

  5
IrNO3 d(N-O)=2.05
   Ir        0.073255   -0.002685    0.004854
   O         0.439984   -0.825985   -1.448877
   O         0.400257   -0.779412    1.493322
   O        -1.389454    1.209321   -0.034412
   N         0.599486    1.705544   -0.014886

  5
IrNO3 d(N-O)=2.00
   Ir        0.054166   -0.013039    0.001143
   O         0.428688   -0.842567   -1.446040
   O         0.138671   -0.861539    1.482933
   O        -1.237312    1.395717   -0.117624
   N         0.739315    1.628212    0.079588

  5
IrNO3 d(N-O)=1.95
   Ir        0.105172   -0.010787    0.006062
   O         0.576024   -0.803010   -1.432479
   O         0.315286   -0.814542    1.498985
   O        -1.373462    1.211558   -0.120822
   N         0.500508    1.723564    0.048255

  5
IrNO3 d(N-O)=1.90
   Ir        0.086898   -0.023795    0.000728
   O         0.713250   -0.769960   -1.401530
   O         0.090411   -0.898046    1.467453
   O        -1.288011    1.294351   -0.239208
   N         0.520979    1.704234    0.172558

  5
IrNO3 d(N-O)=1.85
   Ir        0.101318   -0.027831    0.005208
   O         0.643390   -0.794500   -1.420136
```

```
   O          0.329886   -0.823082    1.497924
   O         -1.354629    1.205226   -0.138673
   N          0.403563    1.746971    0.055677

  5
IrNO3 d(N-O)=1.80
   Ir         0.073774   -0.039889    0.007688
   O          0.412212   -0.886391   -1.434555
   O          0.404723   -0.810810    1.493468
   O         -1.262036    1.326171   -0.030382
   N          0.494855    1.717704   -0.036219

  5
IrNO3 d(N-O)=1.75
   Ir         0.083805   -0.043873    0.004607
   O          0.600914   -0.832739   -1.416723
   O          0.331676   -0.836421    1.494755
   O         -1.285671    1.274729   -0.118756
   N          0.392804    1.745089    0.036116

  5
IrNO3 d(N-O)=1.70
   Ir         0.064358   -0.051976   -0.001853
   O          0.672385   -0.820380   -1.398026
   O          0.153337   -0.907125    1.471325
   O         -1.199128    1.360465   -0.189084
   N          0.432574    1.725800    0.117639

  5
IrNO3 d(N-O)=1.65
   Ir         0.062579   -0.056977    0.003681
   O          0.517081   -0.874014   -1.422859
   O          0.338209   -0.860735    1.482537
   O         -1.199482    1.363328   -0.080198
   N          0.405139    1.735182    0.016839

  5
IrNO3 d(N-O)=1.60
   Ir         0.037313   -0.063391   -0.004403
   O          0.568650   -0.872295   -1.408914
   O          0.133891   -0.929407    1.461935
   O         -1.089325    1.462722   -0.145153
   N          0.473000    1.709154    0.096535

  5
IrNO3 d(N-O)=1.55
   Ir         0.018379   -0.067934    0.000710
   O          0.362738   -0.926711   -1.432514
   O          0.242230   -0.919193    1.462001
   O         -1.019777    1.527150   -0.046926
   N          0.519958    1.693472    0.016729

  5
IrNO3 d(N-O)=1.50
   Ir        -0.006589   -0.070873   -0.009809
   O          0.455431   -0.925601   -1.412520
   O         -0.008892   -0.970509    1.440099
   O         -0.897921    1.611072   -0.129976
   N          0.581499    1.662695    0.112207

  5
IrNO3 d(N-O)=1.45
   Ir        -0.017540   -0.074277   -0.000117
   O          0.205908   -0.961741   -1.440940
   O          0.206169   -0.961373    1.440860
   O         -0.860446    1.642843    0.000061
   N          0.589436    1.661333    0.000135

  5
IrNO3 d(N-O)=1.40
   Ir        -0.020987   -0.078706   -0.000005
   O          0.209845   -0.971755   -1.437506
   O          0.209647   -0.971757    1.437526
   O         -0.837472    1.659627   -0.000064
   N          0.562494    1.669374    0.000048

  5
IrNO3 d(N-O)=1.35
   Ir        -0.075204   -0.073189   -0.000000
   O          0.029900   -0.996451   -1.434258
   O          0.029901   -0.996451    1.434258
   O         -0.598259    1.785276    0.000000
   N          0.737190    1.587600   -0.000000

5
IrNO3 minimum C' d(N-O)=1.315
 Ir        -0.078728 -0.076763 0.000000
 O          0.031763  -1.005077 -1.431833
 O          0.031764  -1.005077 1.431833
 O         -0.580637 1.796744  0.000000
 N          0.719366  1.596957  -0.000000

5
IrN2O2- minimum A d(N-N)=2.777
 Ir        -0.729925 0.260741  -0.161479
 O         -0.134438 1.079120  1.291840
 O         -0.159873 1.093672  -1.616732
 N         -0.167591 -1.350160 -0.174471
 N         -2.436137 0.251239  -0.146615

  5
IrN2O2- d(N-N)=2.74
   Ir        -0.725933    0.266376   -0.161490
   O         -0.131013    1.083925    1.293043
   O         -0.156507    1.098524   -1.617948
   N         -0.188089   -1.347154   -0.174246
   N         -2.426424    0.232942   -0.146815

  5
IrN2O2- d(N-N)=2.69
   Ir        -0.720665    0.273866   -0.161514
   O         -0.105290    1.076303    1.293871
   O         -0.172543    1.120397   -1.618794
   N         -0.216239   -1.343191   -0.197630
   N         -2.413228    0.207237   -0.123390

  5
IrN2O2- d(N-N)=2.64
   Ir        -0.715327    0.281462   -0.161533
   O         -0.082075    1.068739    1.295206
   O         -0.185320    1.139452   -1.619545
   N         -0.245805   -1.338874   -0.217449
   N         -2.399436    0.183832   -0.104137

  5
IrN2O2- d(N-N)=2.59
   Ir        -0.710042    0.288558   -0.161560
   O         -0.078100    1.079054    1.294778
   O         -0.168169    1.135415   -1.622554
   N         -0.284152   -1.338390   -0.206126
   N         -2.387501    0.169974   -0.111994

  5
IrN2O2- d(N-N)=2.54
   Ir        -0.704605    0.295930   -0.161550
   O         -0.074252    1.084267    1.297373
   O         -0.163393    1.142366   -1.623826
   N         -0.311562   -1.333690   -0.206132
   N         -2.374152    0.145739   -0.113322

  5
IrN2O2- d(N-N)=2.49
   Ir        -0.700154    0.303310   -0.161471
   O         -0.069797    1.089984    1.299253
   O         -0.171063    1.159500   -1.623244
   N         -0.326887   -1.325938   -0.213015
   N         -2.360063    0.107755   -0.108979

  5
IrN2O2- d(N-N)=2.44
   Ir        -0.694801    0.310490   -0.161506
   O         -0.065959    1.096368    1.300979
   O         -0.166904    1.165465   -1.625216
   N         -0.354017   -1.321346   -0.212106
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   N        -2.346282    0.083636   -0.109608

  5
IrN2O2- d(N-N)=2.39
   Ir       -0.690399    0.317353   -0.161503
   O        -0.060014    1.103408    1.300964
   O        -0.163872    1.172660   -1.626200
   N        -0.380536   -1.316658   -0.210752
   N        -2.333143    0.057849   -0.109965

  5
IrN2O2- d(N-N)=2.34
   Ir       -0.685378    0.324662   -0.161540
   O        -0.081844    1.127414    1.303940
   O        -0.140453    1.164797   -1.629009
   N        -0.401322   -1.311041   -0.188369
   N        -2.318966    0.028780   -0.132478

  5
IrN2O2- d(N-N)=2.29
   Ir       -0.680399    0.330603   -0.161618
   O        -0.047870    1.113952    1.302743
   O        -0.156112    1.186134   -1.628309
   N        -0.437575   -1.308165   -0.210105
   N        -2.306008    0.012089   -0.110167

  5
IrN2O2- d(N-N)=2.24
   Ir       -0.005183    0.079895    0.000315
   O         0.238753   -0.900139   -1.444542
   O        -0.548657   -0.765814    1.448404
   N        -0.846080    1.620886   -0.300270
   N         1.284694    1.271957    0.296094

  5
IrN2O2- d(N-N)=2.19
   Ir       -0.005850    0.075110    0.000381
   O         0.262069   -0.913457   -1.434441
   O        -0.573413   -0.771283    1.438853
   N        -0.816246    1.627101   -0.312149
   N         1.256967    1.289313    0.307357

  5
IrN2O2- d(N-N)=2.14
   Ir       -0.007116    0.068772    0.000344
   O         0.261173   -0.920171   -1.434025
   O        -0.574411   -0.778016    1.438564
   N        -0.791027    1.633342   -0.304918
   N         1.234907    1.302857    0.300036

  5
IrN2O2- d(N-N)=2.09
   Ir       -0.007550    0.063944    0.000417
   O         0.233893   -0.924356   -1.439377
   O        -0.551086   -0.790405    1.443550
   N        -0.769995    1.641023   -0.280530
   N         1.218265    1.316577    0.275941

  5
IrN2O2- d(N-N)=2.04
   Ir       -0.008344    0.058471    0.000339
   O         0.232509   -0.931260   -1.438565
   O        -0.552025   -0.797281    1.442747
   N        -0.744660    1.646792   -0.273803
   N         1.196046    1.330063    0.269283

  5
IrN2O2- d(N-N)=1.99
   Ir       -0.033908    0.004962   -0.003428
   O         0.124516   -0.944056   -1.466801
   O        -0.597944   -0.819155    1.435279
   N        -0.624517    1.750048   -0.225841
   N         1.255379    1.314984    0.260792

  5
IrN2O2- d(N-N)=1.94
   Ir       -0.037661   -0.011735   -0.003770
   O         0.121112   -0.960722   -1.463506
   O        -0.599162   -0.834733    1.432841
   N        -0.596296    1.769702   -0.221011
   N         1.235533    1.344273    0.255447

  5
IrN2O2- d(N-N)=1.89
   Ir       -0.029807   -0.016873   -0.001927
   O         0.026915   -0.947705   -1.480640
   O        -0.436534   -0.877552    1.464420
   N        -0.634348    1.753387   -0.140168
   N         1.197302    1.395527    0.158316

  5
IrN2O2- d(N-N)=1.84
   Ir       -0.031911   -0.019892   -0.002059
   O        -0.126784   -0.924715   -1.495132
   O        -0.300962   -0.912231    1.477144
   N        -0.608299    1.765362   -0.043872
   N         1.191484    1.398260    0.063920

  5
IrN2O2- d(N-N)=1.79
   Ir       -0.015062   -0.026194   -0.002185
   O        -0.194744   -0.919480   -1.494479
   O        -0.089656   -0.957861    1.475482
   N        -0.674606    1.726511    0.044132
   N         1.097595    1.483808   -0.022948

  5
IrN2O2- d(N-N)=1.74
   Ir       -0.020991   -0.028644   -0.002460
   O        -0.081578   -0.943645   -1.491427
   O        -0.249000   -0.941914    1.471261
   N        -0.620419    1.746279   -0.037221
   N         1.095514    1.474707    0.059848

  5
IrN2O2- d(N-N)=1.69
   Ir        0.009014   -0.035243   -0.001631
   O        -0.022053   -0.957613   -1.487095
   O        -0.061471   -0.970789    1.474260
   N        -0.744739    1.679759   -0.003483
   N         0.942775    1.590670    0.017950

  5
IrN2O2- d(N-N)=1.64
   Ir       -0.002483   -0.037711   -0.001078
   O        -0.197060   -0.953970   -1.478265
   O         0.021562   -0.984679    1.469372
   N        -0.663607    1.715644    0.066055
   N         0.965115    1.567499   -0.056083

  5
IrN2O2- d(N-N)=1.59
   Ir        0.009636   -0.042064   -0.001199
   O         0.014067   -0.979097   -1.478571
   O        -0.088364   -0.985099    1.469182
   N        -0.699445    1.696047   -0.022241
   N         0.887633    1.616997    0.032830

  5
IrN2O2- d(N-N)=1.54
   Ir       -0.004428   -0.044785   -0.000746
   O        -0.201702   -0.974452   -1.470197
   O         0.013752   -1.000983    1.464857
   N        -0.606521    1.736068    0.059734
   N         0.922427    1.590936   -0.053648

  5
IrN2O2- d(N-N)=1.49
   Ir        0.010379   -0.049966   -0.000746
   O         0.013540   -1.001313   -1.470370
   O        -0.082111   -1.003548    1.464586
   N        -0.652939    1.715345   -0.021139
   N         0.834658    1.646266    0.027670
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  5
IrN2O2- d(N-N)=1.44
   Ir       -0.007522   -0.053222   -0.000288
   O        -0.205947   -0.998211   -1.461757
   O        -0.003441   -1.018906    1.461084
   N        -0.544313    1.761595    0.050594
   N         0.884750    1.615528   -0.049631

  5
IrN2O2- d(N-N)=1.39
   Ir        0.004861   -0.059513    0.000077
   O         0.014891   -1.029267   -1.459996
   O        -0.125298   -1.020213    1.460387
   N        -0.578325    1.750813   -0.033778
   N         0.807398    1.664964    0.033311

  5
IrN2O2- d(N-N)=1.34
   Ir       -0.008943   -0.064500   -0.000197
   O        -0.173946   -1.028866   -1.456365
   O        -0.038745   -1.039078    1.458226
   N        -0.493143    1.788405    0.030486
   N         0.838303    1.650823   -0.032149

   5
IrN2O2- d(N-N)=1.29
   Ir        0.015883   -0.073130    0.000000
   O        -0.009939   -1.054207   -1.455631
   O        -0.009938   -1.054206    1.455632
   N        -0.581012    1.761288    0.000000
   N         0.708533    1.727039   -0.000000

5
IrN2O2- minimum C" d(N-N)=1.236
 Ir        0.015453  -0.082705 -0.000000
 O        -0.010337 -1.071590 -1.454241
 O        -0.010336 -1.071589 1.454242
 N        -0.553164 1.782743  -0.000000
 N        0.681911  1.749925  0.000000

5
IrN2O2- minimum A d(N-O)=2.835
 Ir       -0.729925 0.260741  -0.161479
 O        -0.134438 1.079120  1.291840
 O        -0.159873 1.093672  -1.616732
 N        -0.167591 -1.350160 -0.174471
 N        -2.436137 0.251239  -0.146615

  5
IrN2O2- d(N-O)=2.80
   Ir       -0.734216    0.265360   -0.155377
   O        -0.137472    1.082242    1.298463
   O        -0.153497    1.070905   -1.615050
   N        -0.161846   -1.336771   -0.193557
   N        -2.440933    0.252875   -0.141937

  5
IrN2O2- d(N-O)=2.74
   Ir       -0.739801    0.271352   -0.147811
   O        -0.137774    1.095904    1.299813
   O        -0.130636    1.018067   -1.619330
   N        -0.172610   -1.326571   -0.197432
   N        -2.447143    0.275860   -0.142697

  5
IrN2O2- d(N-O)=2.69
   Ir       -0.745312    0.276797   -0.140079
   O        -0.145608    1.098851    1.310171
   O        -0.130568    0.998980   -1.614577
   N        -0.153322   -1.304947   -0.228468
   N        -2.453154    0.264932   -0.134505

  5
IrN2O2- d(N-O)=2.64
   Ir       -0.750907    0.282193   -0.132410
   O        -0.151014    1.101814    1.319561
   O        -0.116676    0.967330   -1.610582
   N        -0.149888   -1.289536   -0.250400
   N        -2.459480    0.272812   -0.133626

  5
IrN2O2- d(N-O)=2.58
   Ir       -0.756242    0.287502   -0.124767
   O        -0.157158    1.100042    1.331781
   O        -0.110164    0.946883   -1.604411
   N        -0.139129   -1.269894   -0.281462
   N        -2.465271    0.270080   -0.128598

  5
IrN2O2- d(N-O)=2.53
   Ir       -0.761829    0.291792   -0.116900
   O        -0.160661    1.101918    1.340586
   O        -0.102008    0.919470   -1.600261
   N        -0.132106   -1.252746   -0.307225
   N        -2.471360    0.274178   -0.123657

  5
IrN2O2- d(N-O)=2.47
   Ir       -0.766796    0.297059   -0.109229
   O        -0.164293    1.104812    1.349247
   O        -0.095033    0.891376   -1.597790
   N        -0.125047   -1.234328   -0.331368
   N        -2.476795    0.275693   -0.118317

  5
IrN2O2- d(N-O)=2.42
   Ir       -0.772614    0.300114   -0.100963
   O        -0.167400    1.130647    1.343969
   O        -0.110147    0.861904   -1.604250
   N        -0.095341   -1.208449   -0.349471
   N        -2.482462    0.250396   -0.096742

  5
IrN2O2- d(N-O)=2.37
   Ir       -0.777293    0.304468   -0.092731
   O        -0.169766    1.131709    1.353254
   O        -0.102965    0.834431   -1.601640
   N        -0.090472   -1.190487   -0.375238
   N        -2.487467    0.254491   -0.091102

  5
IrN2O2- d(N-O)=2.31
   Ir       -0.783188    0.304877   -0.082916
   O        -0.171536    1.130871    1.362484
   O        -0.116119    0.829619   -1.597607
   N        -0.064350   -1.161031   -0.419329
   N        -2.492771    0.230275   -0.070089

  5
IrN2O2- d(N-O)=2.26
   Ir       -0.787807    0.307889   -0.073070
   O        -0.175600    1.133218    1.372269
   O        -0.107439    0.801501   -1.596323
   N        -0.059716   -1.142687   -0.444587
   N        -2.497402    0.234692   -0.065747

  5
IrN2O2- d(N-O)=2.21
   Ir       -0.794692    0.309712   -0.059525
   O        -0.180531    1.164296    1.367555
   O        -0.120973    0.769390   -1.607427
   N        -0.029576   -1.116232   -0.464889
   N        -2.502192    0.207447   -0.043172

5
IrN2O2- TS B' d(N-O)=2.154
 Ir       -0.645825 0.159044  0.025456
 O        -0.081054 0.935391  1.505170
 O        -0.514533 1.185261  -1.616546
 N        -0.137723 -1.446646 -0.183390
 N        -2.248830 0.501563  -0.538146

  5
IrN2O2- d(N-O)=2.10
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```
   Ir        0.024880    0.029205   -0.084410
   O        -1.009609    0.839631   -1.255776
   O        -0.766156   -1.333127    1.120065
   N         1.180915    0.995634    0.683334
   N         0.583562   -1.614902   -0.463211

  5
IrN2O2- d(N-O)=2.05
   Ir        0.041884    0.032905   -0.106758
   O        -0.875045    0.790369   -1.403451
   O        -0.868629   -1.187970    1.172890
   N         1.238753    0.977811    0.619524
   N         0.476630   -1.696675   -0.282204

  5
IrN2O2- d(N-O)=1.99
   Ir        0.024565    0.052468   -0.089938
   O        -1.044048    0.882449   -1.213499
   O        -0.694976   -1.272407    1.208392
   N         1.331294    0.941786    0.500645
   N         0.396758   -1.687856   -0.405598

  5
IrN2O2- d(N-O)=1.94
   Ir        0.032696    0.056483   -0.102526
   O        -0.887992    0.812039   -1.395919
   O        -0.815849   -1.191526    1.182798
   N         1.292917    0.964908    0.552453
   N         0.391822   -1.725463   -0.236804

  5
IrN2O2- d(N-O)=1.89
   Ir        0.019865    0.071599   -0.083461
   O        -1.047581    0.909803   -1.200473
   O        -0.650064   -1.269807    1.206419
   N         1.380540    0.922557    0.429947
   N         0.310832   -1.717712   -0.352430

  5
IrN2O2- d(N-O)=1.83
   Ir        0.022303    0.075728   -0.092232
   O        -0.877138    0.830050   -1.400580
   O        -0.781664   -1.236106    1.136625
   N         1.285898    0.978735    0.559692
   N         0.364194   -1.731968   -0.203504

  5
IrN2O2- d(N-O)=1.78
   Ir        0.011558    0.087950   -0.071825
   O        -1.039567    0.927081   -1.203347
   O        -0.621373   -1.312201    1.153015
   N         1.372732    0.937234    0.439214
   N         0.290243   -1.723625   -0.317056

  5
IrN2O2- d(N-O)=1.72
   Ir        0.010126    0.092392   -0.076501
   O        -0.898970    0.868374   -1.365628
   O        -0.718141   -1.316956    1.071462
   N         1.264899    0.999192    0.584861
   N         0.355678   -1.726563   -0.214191

  5
IrN2O2- d(N-O)=1.67
   Ir        0.005515    0.100893   -0.063126
   O        -1.034205    0.940788   -1.206050
   O        -0.588463   -1.350738    1.104645
   N         1.365196    0.953787    0.445519
   N         0.265550   -1.728290   -0.280986

  5
IrN2O2- d(N-O)=1.62
   Ir        0.003752    0.108366   -0.049985
   O        -1.148836    1.013534   -1.022956
   O        -0.460388   -1.390003    1.115649
   N         1.444716    0.909217    0.291055
   N         0.174349   -1.724674   -0.333761

  5
IrN2O2- d(N-O)=1.56
   Ir        0.006809    0.114580   -0.040081
   O        -1.233292    1.079414   -0.832865
   O        -0.334888   -1.417171    1.123946
   N         1.508300    0.862496    0.105106
   N         0.066664   -1.722880   -0.356105

  5
IrN2O2- d(N-O)=1.51
   Ir        0.005987    0.122047   -0.010839
   O        -1.294662    1.154640   -0.596471
   O        -0.224417   -1.517798    1.033027
   N         1.523654    0.851185    0.023795
   N         0.003031   -1.693634   -0.449509

  5
IrN2O2- d(N-O)=1.46
   Ir        0.008284    0.126420    0.024488
   O        -1.331414    1.213922   -0.333791
   O        -0.130191   -1.622885    0.900304
   N         1.528203    0.850401   -0.036637
   N        -0.061290   -1.651418   -0.554362

  5
IrN2O2- d(N-O)=1.40
   Ir        0.012916    0.125578    0.072003
   O        -1.342919    1.247732   -0.046921
   O        -0.066548   -1.736692    0.699612
   N         1.526348    0.860383   -0.030903
   N        -0.116205   -1.580561   -0.693789

5
IrN2O2- minimum N-O d(N-O)=1.366
 Ir        0.013241  0.128690  0.073423
 O        -1.341376 1.254027  -0.048369
 O        -0.066996 -1.744905 0.683240
 N         1.525493  0.866857  -0.031560
 N        -0.116769 -1.588229 -0.676732

5
IrN2O2- minimum A d(O-O)=2.904
 Ir       -0.729925 0.260741  -0.161479
 O        -0.134438 1.079120  1.291840
 O        -0.159873 1.093672  -1.616732
 N        -0.167591 -1.350160 -0.174471
 N        -2.436137 0.251239  -0.146615

  5
IrN2O2- d(O-O)=2.85
   Ir       -0.737018    0.250682   -0.161473
   O        -0.123901    1.094503    1.260462
   O        -0.148875    1.108814   -1.585393
   N        -0.174441   -1.360660   -0.174399
   N        -2.443729    0.241274   -0.146654

  5
IrN2O2- d(O-O)=2.79
   Ir       -0.743532    0.241436   -0.161463
   O        -0.136064    1.121648    1.233734
   O        -0.119185    1.106572   -1.558636
   N        -0.178649   -1.369367   -0.149336
   N        -2.450534    0.234323   -0.171755

  5
IrN2O2- d(O-O)=2.74
   Ir       -0.749737    0.232641   -0.161437
   O        -0.143757    1.146777    1.205928
   O        -0.094477    1.106716   -1.532259
   N        -0.183065   -1.377690   -0.127622
   N        -2.456928    0.226168   -0.192067

  5
IrN2O2- d(O-O)=2.69
   Ir       -0.755661    0.224320   -0.161364
   O        -0.126705    1.154645    1.178158
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   O        -0.092966    1.122086   -1.506817
   N        -0.189513   -1.386453   -0.134548
   N        -2.463119    0.220014   -0.182887

  5
IrN2O2- d(O-O)=2.63
   Ir       -0.761705    0.215832   -0.161323
   O        -0.117460    1.166179    1.151297
   O        -0.083846    1.133666   -1.480133
   N        -0.195217   -1.395426   -0.134584
   N        -2.469736    0.214361   -0.182714

  5
IrN2O2- d(O-O)=2.58
   Ir       -0.767564    0.207575   -0.161322
   O        -0.108635    1.177083    1.124529
   O        -0.076615    1.146020   -1.453392
   N        -0.199497   -1.403181   -0.133810
   N        -2.475653    0.207114   -0.183462

  5
IrN2O2- d(O-O)=2.52
   Ir       -0.773120    0.199684   -0.161262
   O        -0.100684    1.188823    1.097693
   O        -0.068099    1.157403   -1.426671
   N        -0.204333   -1.411378   -0.134856
   N        -2.481728    0.200080   -0.182361

  5
IrN2O2- d(O-O)=2.47
   Ir       -0.778922    0.191764   -0.160820
   O        -0.093321    1.207112    1.065593
   O        -0.056876    1.159222   -1.404905
   N        -0.211198   -1.419586   -0.120409
   N        -2.487647    0.196101   -0.186915

  5
IrN2O2- d(O-O)=2.42
   Ir       -0.784249    0.184282   -0.160756
   O        -0.081025    1.214556    1.038911
   O        -0.053567    1.173692   -1.378280
   N        -0.215634   -1.427373   -0.127657
   N        -2.493490    0.189455   -0.179674

  5
IrN2O2- d(O-O)=2.36
   Ir       -0.789160    0.176554   -0.160486
   O        -0.074160    1.224840    1.012690
   O        -0.046098    1.185206   -1.350965
   N        -0.220348   -1.435080   -0.126370
   N        -2.498198    0.183092   -0.182325

  5
IrN2O2- d(O-O)=2.31
   Ir       -0.794621    0.169842   -0.160424
   O        -0.047422    1.223972    0.983651
   O        -0.057457    1.206408   -1.326876
   N        -0.224134   -1.441872   -0.151522
   N        -2.504330    0.176262   -0.152287

  5
IrN2O2- d(O-O)=2.26
   Ir       -0.799521    0.162608   -0.160756
   O        -0.059998    1.244970    0.959069
   O        -0.030417    1.206002   -1.297478
   N        -0.228833   -1.448780   -0.123604
   N        -2.509195    0.169811   -0.184688

  5
IrN2O2- d(O-O)=2.20
   Ir       -0.007725   -0.001276   -0.046919
   O         0.835070   -0.700674    1.467428
   O        -0.854147    0.714258    1.457804
   N        -0.920386   -1.097652   -0.978952
   N         0.907150    1.085086   -0.988468

  5
IrN2O2- d(O-O)=2.15
   Ir       -0.007721   -0.001303   -0.052464
   O         0.826194   -0.669403    1.476671
   O        -0.845164    0.682993    1.467540
   N        -0.900321   -1.112509   -0.985555
   N         0.886974    1.099964   -0.995298

  5
IrN2O2- d(O-O)=2.10
   Ir       -0.007720   -0.001330   -0.057968
   O         0.813134   -0.642770    1.485623
   O        -0.832181    0.656466    1.476781
   N        -0.887380   -1.122224   -0.991862
   N         0.874108    1.109600   -1.001680

  5
IrN2O2- d(O-O)=2.04
   Ir       -0.007719   -0.001348   -0.063005
   O         0.788764   -0.630364    1.494037
   O        -0.807834    0.644130    1.485412
   N        -0.892436   -1.117461   -0.997905
   N         0.879186    1.104786   -1.007646

  5
IrN2O2- d(O-O)=1.99
   Ir       -0.007709   -0.001376   -0.067967
   O         0.767983   -0.613427    1.502289
   O        -0.787079    0.627284    1.493902
   N        -0.892147   -1.116870   -1.003797
   N         0.878914    1.104130   -1.013534

  5
IrN2O2- d(O-O)=1.94
   Ir       -0.007586   -0.001467   -0.073000
   O         0.745011   -0.599212    1.510312
   O        -0.764174    0.613138    1.502068
   N        -0.890223   -1.117895   -1.009336
   N         0.876934    1.105178   -1.019151

  5
IrN2O2- d(O-O)=1.88
   Ir       -0.008321   -0.001194   -0.138587
   O         0.809969   -0.473077    1.580104
   O        -0.814232    0.478212    1.590179
   N        -0.733862   -1.235173   -1.054946
   N         0.706407    1.230974   -1.065857

  5
IrN2O2- d(O-O)=1.83
   Ir       -0.009523   -0.000755   -0.158600
   O         0.787526   -0.459758    1.611594
   O        -0.790043    0.465243    1.618396
   N        -0.736029   -1.232533   -1.074421
   N         0.708031    1.227545   -1.086076

  5
IrN2O2- d(O-O)=1.78
   Ir       -0.008239   -0.001466   -0.162229
   O         0.793307   -0.377216    1.621649
   O        -0.808041    0.389026    1.620046
   N        -0.619325   -1.293723   -1.078734
   N         0.602259    1.283121   -1.089839

  5
IrN2O2- d(O-O)=1.72
   Ir       -0.008983   -0.001300   -0.166034
   O         0.818197   -0.251499    1.625062
   O        -0.825387    0.261181    1.629313
   N        -0.433520   -1.365908   -1.082913
   N         0.409654    1.357268   -1.094535

  5
IrN2O2- d(O-O)=1.67
   Ir       -0.008676   -0.001492   -0.169762
   O         0.815436   -0.140446    1.632087
   O        -0.827013    0.151263    1.634357
   N        -0.258304   -1.408086   -1.087571
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   N         0.238518    1.398503   -1.098218

  5
IrN2O2- d(O-O)=1.61
   Ir        0.001810   -0.001873   -0.173748
   O         0.764291    0.007353    1.657879
   O        -0.849833    0.007540    1.618037
   N         0.021453   -1.432454   -1.088275
   N         0.022239    1.419176   -1.103000

  5
IrN2O2- d(O-O)=1.56
   Ir        0.000782   -0.001890   -0.177388
   O         0.737389    0.007168    1.662006
   O        -0.823246    0.007773    1.624860
   N         0.021668   -1.432546   -1.091943
   N         0.023368    1.419237   -1.106641

  5
IrN2O2- d(O-O)=1.51
   Ir        0.000752   -0.001919   -0.181077
   O         0.710503    0.007290    1.667300
   O        -0.796608    0.007727    1.631422
   N         0.022061   -1.432439   -1.096035
   N         0.023254    1.419083   -1.110718

   5
IrN2O2- d(O-O)=1.45
   Ir        0.000218   -0.001937   -0.185079
   O         0.685882    0.005529    1.671367
   O        -0.767747    0.009546    1.638770
   N         0.016732   -1.432896   -1.099809
   N         0.024876    1.419501   -1.114356

5
IrN2O2- minimum C d(O-O)=1.445
 Ir        0.000230  -0.001941 -0.185816
 O         0.681443  0.005545  1.672044
 O         -0.763344 0.009538  1.639654
 N         0.016743  -1.433110 -1.100220
 N         0.024889  1.419710  -1.114769

5
PtO4_2+ minimum A d(O-O)=2.794  1
 Pt        0.000000  0.000037  -0.021394
 O         -1.397059 -0.806621 0.548956
 O         1.397057  -0.806621 0.548961
 O         -0.000001 1.613228  0.548971
 O         0.000004  -0.000021 -1.732471

  5
PtO4_2+ d(O-O)=2.75
   Pt       -0.000004   -0.008166   -0.015676
   O        -1.398022   -0.813065    0.553344
   O         1.397914   -0.822156    0.540506
   O         0.007762    1.606516    0.536416
   O        -0.007647    0.036872   -1.721566

  5
PtO4_2+ d(O-O)=2.70
   Pt        0.000006   -0.017059   -0.009483
   O        -1.398742   -0.815986    0.565101
   O         1.398434   -0.835086    0.538374
   O         0.015980    1.603977    0.508338
   O        -0.015677    0.064155   -1.709306

  5
PtO4_2+ d(O-O)=2.68
   Pt        0.000599   -0.141634    0.081289
   O        -1.470393   -0.850745    0.626875
   O         1.477882   -0.872591    0.578941
   O         0.019419    1.717116    0.385876
   O        -0.027506    0.147853   -1.779957

  5
PtO4_2+ d(O-O)=2.65
   Pt        0.000610   -0.143335    0.082827
   O        -1.467510   -0.856777    0.628770
   O         1.475077   -0.874756    0.586258
   O         0.016106    1.716133    0.369427
   O        -0.024282    0.158736   -1.774258

  5
PtO4_2+ d(O-O)=2.63
   Pt        0.000634   -0.146761    0.085647
   O        -1.467484   -0.858232    0.632686
   O         1.475156   -0.877219    0.588716
   O         0.016642    1.713907    0.353649
   O        -0.024947    0.168306   -1.767674

  5
PtO4_2+ d(O-O)=2.60
   Pt        0.000662   -0.148188    0.086641
   O        -1.464552   -0.862675    0.636780
   O         1.472247   -0.882842    0.591305
   O         0.017387    1.712017    0.339891
   O        -0.025742    0.181688   -1.761593

  5
PtO4_2+ minimum d(O-O)=2.575
   Pt        0.000683   -0.151474    0.088803
   O        -1.464071   -0.865367    0.639156
   O         1.471751   -0.886714    0.592165
   O         0.018084    1.708875    0.327586
   O        -0.026446    0.194680   -1.754686

  5
PtO4_2+ d(O-O)=2.55
   Pt        0.000688   -0.153121    0.090145
   O        -1.461789   -0.869540    0.642900
   O         1.469545   -0.890562    0.596323
   O         0.017629    1.707141    0.312290
   O        -0.026071    0.206081   -1.748634

  5
PtO4_2+ d(O-O)=2.53
   Pt        0.000691   -0.156129    0.092284
   O        -1.461416   -0.872488    0.644903
   O         1.469199   -0.893346    0.598528
   O         0.017282    1.704119    0.299042
   O        -0.025756    0.217844   -1.741733

  5
PtO4_2+ d(O-O)=2.50
   Pt        0.000690   -0.157680    0.093407
   O        -1.458721   -0.877386    0.647669
   O         1.466546   -0.897499    0.602352
   O         0.016349    1.702075    0.285088
   O        -0.024863    0.230491   -1.735492

5
PtO4_2+ d(O-O)=2.47
 Pt        0.000734  -0.160728 0.095509
 O         -1.458054 -0.888156 0.640232
 O         1.466182  -0.894252 0.613521
 O         0.006165  1.698607  0.271514
 O         -0.015026 0.244528  -1.727751

  5
PtO4_2+ d(O-O)=2.45
   Pt        0.000705   -0.162621    0.096996
   O        -1.455841   -0.894495    0.640625
   O         1.464041   -0.896609    0.619442
   O         0.010032    1.697324    0.258612
   O        -0.018936    0.256401   -1.722651

  5
PtO4_2+ d(O-O)=2.40
   Pt        0.000739   -0.166670    0.099701
   O        -1.454018   -0.890931    0.657866
   O         1.462147   -0.913132    0.609129
   O         0.018060    1.690318    0.234008
   O        -0.026926    0.280415   -1.707680
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  5
PtO4_2+ d(O-O)=2.35
   Pt        0.000774   -0.170979    0.102777
   O        -1.451219   -0.899909    0.659922
   O         1.459438   -0.918196    0.616574
   O         0.013355    1.684624    0.207713
   O        -0.022346    0.304460   -1.693963

  5
PtO4_2+ d(O-O)=2.30
   Pt        0.000787   -0.176509    0.106167
   O        -1.451012   -0.922379    0.640146
   O         1.459173   -0.909541    0.639894
   O        -0.008010    1.677451    0.185739
   O        -0.000936    0.330978   -1.678922

  5
PtO4_2+ d(O-O)=2.25
   Pt        0.000797   -0.179679    0.108200
   O        -1.445026   -0.918826    0.666292
   O         1.453291   -0.934265    0.627064
   O         0.011625    1.674202    0.158225
   O        -0.020686    0.358567   -1.666757

  5
PtO4_2+ d(O-O)=2.20
   Pt        0.000765   -0.183849    0.111838
   O        -1.444201   -0.937209    0.653220
   O         1.452196   -0.924929    0.652964
   O        -0.007321    1.668177    0.128416
   O        -0.001439    0.377810   -1.653414

  5
PtO4_2+ d(O-O)=2.15
   Pt        0.000780   -0.185996    0.113313
   O        -1.437993   -0.953952    0.650868
   O         1.446087   -0.927879    0.669627
   O        -0.015591    1.664360    0.100261
   O         0.006718    0.403467   -1.641046

  5
PtO4_2+ d(O-O)=2.10
   Pt        0.000365   -0.189370    0.115958
   O        -1.434383   -0.962945    0.657623
   O         1.442463   -0.936684    0.675768
   O        -0.015079    1.660321    0.072218
   O         0.006636    0.428679   -1.628543

  5
PtO4_2+ d(O-O)=2.05
   Pt        0.000458   -0.193818    0.118749
   O        -1.433223   -0.969928    0.659728
   O         1.441507   -0.940905    0.681400
   O        -0.018987    1.653074    0.046943
   O         0.010245    0.451577   -1.613796

  5
PtO4_2+ d(O-O)=2.00
   Pt        0.000681   -0.196073    0.121086
   O        -1.426364   -0.993033    0.652600
   O         1.435113   -0.939890    0.707423
   O        -0.028642    1.651475    0.015208
   O         0.019212    0.477521   -1.603292

  5
PtO4_2+ d(O-O)=1.95
   Pt       -0.004711   -0.199195    0.124584
   O        -1.420617   -1.003753    0.668545
   O         1.427815   -0.949762    0.709901
   O        -0.022214    1.650205   -0.017042
   O         0.019728    0.502505   -1.592963

  5
PtO4_2+ d(O-O)=1.90
   Pt        0.001097   -0.247576    0.158505
   O        -1.453548   -0.980610    0.634079
   O         1.461293   -0.906563    0.717942
   O        -0.041330    1.632044   -0.045674
   O         0.032489    0.502705   -1.571828

  5
PtO4_2+ d(O-O)=1.85
   Pt       -0.000005   -0.253125    0.165580
   O        -1.452013   -0.986388    0.638463
   O         1.459470   -0.911694    0.720197
   O        -0.040593    1.624789   -0.072196
   O         0.033142    0.526418   -1.559020

  5
PtO4_2+ d(O-O)=1.80
   Pt        0.032134   -0.349311    0.023359
   O        -0.273027   -1.386924   -1.343051
   O        -0.273377   -1.208366    1.511449
   O        -0.053897    2.943872   -0.135977
   O         0.691690    1.307514   -0.055778

  5
PtO4_2+ d(O-O)=1.75
   Pt        0.062311   -0.331041    0.012512
   O        -0.246990   -1.343292   -1.371153
   O        -0.123851   -1.241966    1.487081
   O        -0.242369    2.856859   -0.065331
   O         0.674423    1.366226   -0.063107

  5
PtO4_2+ d(O-O)=1.70  9
   Pt        0.072811   -0.320061    0.017387
   O        -0.219202   -1.324945   -1.373715
   O        -0.109695   -1.227718    1.491530
   O        -0.312840    2.775200   -0.071263
   O         0.692449    1.404309   -0.063937

  5
PtO4_2+ d(O-O)=1.65
   Pt        0.078690   -0.315019    0.017307
   O        -0.230590   -1.308400   -1.375872
   O        -0.122467   -1.211832    1.493335
   O        -0.328110    2.705712   -0.068615
   O         0.726001    1.436325   -0.066153

  5
PtO4_2+ d(O-O)=1.60
   Pt        0.100231   -0.316610    0.016518
   O        -0.191307   -1.305361   -1.381062
   O        -0.082858   -1.208488    1.495354
   O        -0.406083    2.644974   -0.063845
   O         0.703541    1.492270   -0.066964

  5
PtO4_2+ d(O-O)=1.55
   Pt        0.114659   -0.324169    0.015727
   O        -0.203992   -1.307989   -1.376067
   O        -0.095145   -1.209846    1.491656
   O        -0.400559    2.615763   -0.062793
   O         0.708560    1.533025   -0.068522

  5
PtO4_2+ d(O-O)=1.50
   Pt        0.112551   -0.330184    0.016654
   O        -0.197527   -1.318547   -1.372079
   O        -0.090421   -1.220415    1.489093
   O        -0.392535    2.606362   -0.064215
   O         0.691455    1.569569   -0.069451

  5
PtO4_2+ d(O-O)=1.45
   Pt        0.108018   -0.339986    0.016835
   O        -0.193869   -1.331555   -1.370782
   O        -0.086715   -1.232454    1.488345
   O        -0.370031    2.612555   -0.064736
   O         0.666120    1.598225   -0.069659

  5
PtO4_2+ d(O-O)=1.40
```

```
   Pt         0.106479   -0.348016    0.016797
   O         -0.191142   -1.341578   -1.369763
   O         -0.083022   -1.242313    1.487399
   O         -0.350950    2.612734   -0.065704
   O          0.642158    1.625958   -0.068728

  5
PtO4_2+ d(O-O)=1.35
   Pt         0.098788   -0.356009    0.015918
   O         -0.180395   -1.357194   -1.369117
   O         -0.063187   -1.259212    1.484829
   O         -0.335765    2.624158   -0.066505
   O          0.604082    1.655042   -0.065123

  5
PtO4_2+ d(O-O)=1.30
   Pt         0.087354   -0.366527    0.021711
   O         -0.177267   -1.369670   -1.366820
   O         -0.076696   -1.273208    1.488890
   O         -0.293448    2.637886   -0.074491
   O          0.583580    1.678305   -0.069288

  5
PtO4_2+ d(O-O)=1.26
   Pt        -0.003429   -0.382109   -0.029823
   O         -0.423610   -1.430720   -1.345432
   O         -0.228987   -1.173089    1.497406
   O          0.042973    2.672265   -0.054481
   O          0.736577    1.620438   -0.067668

  5
PtO4_2+ d(O-O)=1.24
   Pt         0.002806   -0.391488   -0.034187
   O         -0.368699   -1.470246   -1.340411
   O         -0.217585   -1.167303    1.503576
   O          0.010367    2.684124   -0.078028
   O          0.696636    1.651699   -0.050948

  5
PtO4_2+ d(O-O)=1.22
   Pt         0.000124   -0.408912   -0.075803
   O         -0.380048   -1.539908   -1.336117
   O         -0.208102   -1.129798    1.491818
   O          0.025153    2.705259   -0.048564
   O          0.686396    1.680144   -0.031331

  5
PtO4_2+ d(O-O)=1.20
   Pt        -0.004814   -0.419930   -0.051594
   O         -0.397123   -1.503320   -1.350261
   O         -0.174981   -1.191018    1.496815
   O          0.029250    2.717402   -0.040112
   O          0.671193    1.703651   -0.054846

  5
PtO4_2+ d(O-O)=1.18
   Pt        -0.004786   -0.445279   -0.034109
   O         -0.403010   -1.506259   -1.351489
   O         -0.179004   -1.240376    1.502475
   O          0.040071    2.748134   -0.064082
   O          0.670252    1.750565   -0.052793

5
PtNO3+ minimum A d(O-O)=2.846
 Pt         0.000000  0.000034  -0.008077
 O         -1.423049 -0.821621  0.535944
 O          1.423049  -0.821622 0.535945
 O         -0.000000 1.643229   0.535962
 N          0.000000  -0.000020 -1.706752

  5
PtNO3+ d(O-O)=2.80
   Pt        -0.007777   -0.004490   -0.013237
   O         -1.430235   -0.825708    0.531361
   O          1.421858   -0.795677    0.543280
   O          0.021819    1.629172    0.543314
   N         -0.005665   -0.003296   -1.711697

  5
PtNO3+ d(O-O)=2.75
   Pt        -0.016238   -0.009368   -0.018185
   O         -1.434970   -0.829814    0.535439
   O          1.424574   -0.763549    0.547548
   O          0.047142    1.616613    0.544773
   N         -0.020508   -0.013883   -1.716552

  5
PtNO3+ d(O-O)=2.70
   Pt        -0.024481   -0.013923   -0.023390
   O         -1.453181   -0.813228    0.534066
   O          1.413225   -0.741153    0.572109
   O          0.083014    1.608081    0.531650
   N         -0.018577   -0.039778   -1.721413

  5
PtNO3+ d(O-O)=2.65
   Pt        -0.032434   -0.018624   -0.028589
   O         -1.457837   -0.821238    0.530930
   O          1.414307   -0.712110    0.574130
   O          0.104258    1.591218    0.543223
   N         -0.028294   -0.039246   -1.726672

  5
PtNO3+ d(O-O)=2.60
   Pt        -0.040271   -0.022956   -0.033307
   O         -1.464804   -0.826199    0.526551
   O          1.412980   -0.683780    0.581120
   O          0.128078    1.576321    0.549989
   N         -0.035983   -0.043385   -1.731330

  5
PtNO3+ d(O-O)=2.55
   Pt        -0.047806   -0.027278   -0.038568
   O         -1.471948   -0.830087    0.521622
   O          1.410185   -0.656157    0.589215
   O          0.150119    1.560534    0.557348
   N         -0.040549   -0.047012   -1.736595

  5
PtNO3+ d(O-O)=2.50
   Pt        -0.055079   -0.031841   -0.042641
   O         -1.484805   -0.822913    0.519169
   O          1.404984   -0.626886    0.606150
   O          0.176203    1.549589    0.550844
   N         -0.041303   -0.067950   -1.740500

  5
PtNO3+ d(O-O)=2.50
   Pt        -0.148775   -0.087611   -0.093649
   O         -1.526879   -0.922719    0.538745
   O          1.518558   -0.560157    0.593115
   O          0.236075    1.585461    0.632669
   N         -0.078980   -0.014973   -1.777858

  5
PtNO3+ d(O-O)=2.45
   Pt        -0.153803   -0.090750   -0.095934
   O         -1.533147   -0.927796    0.528894
   O          1.513582   -0.532389    0.602016
   O          0.255077    1.569360    0.638289
   N         -0.081709   -0.018424   -1.780244

  5
PtNO3+ d(O-O)=2.40
   Pt        -0.158465   -0.093529   -0.097884
   O         -1.538143   -0.930095    0.525076
   O          1.509527   -0.505243    0.607441
   O          0.276866    1.553742    0.641044
   N         -0.089786   -0.024874   -1.782654

  5
PtNO3+ d(O-O)=2.35
   Pt        -0.162861   -0.096188   -0.099972
   O         -1.543049   -0.934286    0.518304
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   O         1.505414   -0.478722    0.612302
   O         0.297234    1.536611    0.647413
   N        -0.096738   -0.027413   -1.785026

  5
PtNO3+ d(O-O)=2.30
   Pt       -0.167885   -0.097194   -0.102175
   O        -1.563541   -0.910639    0.512998
   O         1.491023   -0.466857    0.629949
   O         0.335096    1.521543    0.639964
   N        -0.094693   -0.046853   -1.787713

  5
PtNO3+ d(O-O)=2.30
   Pt       -0.167944   -0.097251   -0.102165
   O        -1.563628   -0.910551    0.512915
   O         1.491149   -0.466780    0.629818
   O         0.335074    1.521532    0.640052
   N        -0.094651   -0.046949   -1.787598

  5
PtNO3+ d(O-O)=2.25
   Pt       -0.171398   -0.099974   -0.105588
   O        -1.575114   -0.899934    0.507782
   O         1.477040   -0.437478    0.655855
   O         0.354319    1.512164    0.625957
   N        -0.084848   -0.074778   -1.790984

  5
PtNO3+ d(O-O)=2.20
   Pt       -0.176265   -0.102782   -0.104446
   O        -1.584065   -0.891458    0.512543
   O         1.473798   -0.408470    0.661115
   O         0.382441    1.501185    0.614645
   N        -0.095909   -0.098474   -1.790834

  5
PtNO3+ d(O-O)=2.15
   Pt       -0.179999   -0.104920   -0.107708
   O        -1.583824   -0.900361    0.508665
   O         1.470212   -0.383403    0.659685
   O         0.399194    1.480555    0.626812
   N        -0.105584   -0.091871   -1.794432

  5
PtNO3+ d(O-O)=2.10
   Pt       -0.184173   -0.107321   -0.106593
   O        -1.592779   -0.893313    0.510208
   O         1.466558   -0.354200    0.666609
   O         0.426751    1.469631    0.617198
   N        -0.116357   -0.114798   -1.794400

  5
PtNO3+ d(O-O)=2.05
   Pt       -0.188511   -0.109785   -0.110178
   O        -1.604473   -0.882746    0.504608
   O         1.453663   -0.329758    0.683174
   O         0.447079    1.454708    0.612677
   N        -0.107758   -0.132420   -1.797258

  5
PtNO3+ d(O-O)=2.00
   Pt       -0.191155   -0.111356   -0.110216
   O        -1.602389   -0.898814    0.496977
   O         1.455018   -0.302799    0.676534
   O         0.464962    1.434295    0.628659
   N        -0.126437   -0.121326   -1.798933

  5
PtNO3+ d(O-O)=1.97
   Pt       -0.023238    0.066201    0.015453
   O        -1.306809    1.185908    0.288788
   O         0.027405   -1.562643   -0.988999
   O        -0.167539   -1.530269    0.966832
   N         1.483774    0.757242   -0.282072

  5
PtNO3+ d(O-O)=1.92
   Pt       -0.030599    0.085198    0.000479
   O        -1.338748    1.204707    0.077284
   O         0.172984   -1.612506   -0.912306
   O        -0.303318   -1.506629    0.943029
   N         1.513275    0.745670   -0.108484

  5
PtNO3+ d(O-O)=1.87
   Pt       -0.032787    0.096982    0.004356
   O        -1.339978    1.210471    0.137211
   O         0.134506   -1.608660   -0.916671
   O        -0.258465   -1.532497    0.911062
   N         1.510317    0.750142   -0.135956

  5
PtNO3+ d(O-O)=1.87
   Pt       -0.251188   -0.152268   -0.136278
   O        -1.578376   -1.045507    0.501973
   O         1.344516   -0.257276    0.847874
   O         0.662912    1.446556    0.488328
   N        -0.177864    0.008496   -1.808875

  5
PtNO3+ d(O-O)=1.86
   Pt       -0.254160   -0.152312   -0.137071
   O        -1.566021   -1.068718    0.499542
   O         1.354031   -0.255813    0.830371
   O         0.661428    1.439916    0.507253
   N        -0.195279    0.036927   -1.807073

  5
PtNO3+ d(O-O)=1.85
   Pt       -0.256307   -0.153638   -0.137983
   O        -1.568516   -1.068534    0.499593
   O         1.357040   -0.249513    0.825003
   O         0.661582    1.436352    0.514046
   N        -0.193799    0.035333   -1.807638

  5
PtNO3+ d(O-O)=1.83
   Pt       -0.021873    0.102079    0.007193
   O        -1.335420    1.208924    0.077848
   O        -0.099313   -1.576108   -0.937228
   O        -0.028778   -1.612841    0.891044
   N         1.498978    0.794387   -0.038856

  5
PtNO3+ d(O-O)=1.82
   Pt       -0.022270    0.102797    0.006842
   O        -1.335056    1.210433    0.078553
   O        -0.098668   -1.579221   -0.932630
   O        -0.028978   -1.612920    0.885723
   N         1.498567    0.795351   -0.038487

  5
PtNO3+ d(O-O)=1.78
   Pt       -0.022733    0.106019   -0.004078
   O        -1.331147    1.218080   -0.083140
   O        -0.014348   -1.610067   -0.882224
   O        -0.114938   -1.595837    0.891185
   N         1.496760    0.798244    0.078258

  5
PtNO3+ d(O-O)=1.73
   Pt       -0.023364    0.109744   -0.003017
   O        -1.330496    1.225301    0.033948
   O        -0.097658   -1.621267   -0.846037
   O        -0.031574   -1.599416    0.881509
   N         1.496686    0.802076   -0.066403

  5
PtNO3+ d(O-O)=1.68
   Pt       -0.023431    0.113394    0.003447
   O        -1.315921    1.232750    0.177473
   O        -0.178909   -1.618328   -0.821016
   O         0.048313   -1.616907    0.845140
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   N         1.483542    0.805530   -0.205042

  5
PtNO3+ d(O-O)=1.63
   Pt       -0.024184    0.117049    0.002667
   O        -1.316567    1.240217    0.150765
   O        -0.162006   -1.626067   -0.800462
   O         0.030284   -1.625032    0.822396
   N         1.486067    0.810271   -0.175365

  5
PtNO3+ d(O-O)=1.59
   Pt       -0.024978    0.120876    0.000386
   O        -1.322439    1.247459    0.042620
   O        -0.094332   -1.634449   -0.786952
   O        -0.038374   -1.633231    0.798903
   N         1.493717    0.815784   -0.054955

  5
PtNO3+ d(O-O)=1.54
   Pt       -0.025238    0.124204   -0.001414
   O        -1.319652    1.254419   -0.049929
   O        -0.037434   -1.644233   -0.768228
   O        -0.095934   -1.640684    0.770129
   N         1.491852    0.822733    0.049443

  5
PtNO3+ d(O-O)=1.49
   Pt       -0.025796    0.129059   -0.001721
   O        -1.319185    1.261977   -0.015191
   O        -0.060398   -1.654846   -0.742195
   O        -0.073014   -1.647828    0.749840
   N         1.491987    0.828077    0.009267

  5
PtNO3+ d(O-O)=1.44
   Pt       -0.026160    0.133283    0.002080
   O        -1.310061    1.270089    0.136444
   O        -0.143650   -1.662817   -0.706036
   O         0.011514   -1.658653    0.730338
   N         1.481951    0.834537   -0.162825

  5
PtNO3+ d(O-O)=1.40
   Pt       -0.026469    0.138328    0.000126
   O        -1.310881    1.283688    0.004705
   O        -0.073173   -1.671278   -0.698571
   O        -0.068256   -1.671425    0.698788
   N         1.492373    0.837126   -0.005047

5
PtNO3+ minimum C' d(O-O)=1.355
 Pt        -0.026583 0.142982  0.000154
 O         -1.308729 1.292517  0.004692
 O         -0.073445 -1.682362 -0.677165
 O         -0.068703 -1.682523 0.677379
 N         1.491054  0.845825  -0.005059

5
PtNO3+ minimum A d(N-O)=2.780  9
 Pt        0.000000  0.000034  -0.008077
 O         -1.423049 -0.821621 0.535944
 O         1.423049  -0.821622 0.535945
 O         -0.000000 1.643229  0.535962
 N         0.000000  -0.000020 -1.706752

  5
PtNO3+ d(N-O)=2.75  6
   Pt        0.000006   -0.005508   -0.003710
   O        -1.425315   -0.824815    0.537899
   O         1.425318   -0.824858    0.537857
   O        -0.000035    1.640398    0.519528
   N         0.000026    0.014782   -1.698551

  5
PtNO3+ d(N-O)=2.70  1
   Pt       -0.000017   -0.013153    0.002464
   O        -1.424029   -0.845056    0.525994
   O         1.423437   -0.843404    0.530112
   O        -0.001757    1.629688    0.519878
   N         0.002366    0.071926   -1.685426

  5
PtNO3+ d(N-O)=2.65
   Pt        0.000126   -0.021209    0.009157
   O        -1.425395   -0.836261    0.553346
   O         1.424356   -0.850102    0.535531
   O         0.010893    1.634121    0.468285
   N        -0.009979    0.073451   -1.673297

  5
PtNO3+ d(N-O)=2.60
   Pt        0.000082   -0.028715    0.015195
   O        -1.424157   -0.845655    0.559287
   O         1.425507   -0.856633    0.539208
   O         0.009766    1.631578    0.439912
   N        -0.011198    0.099425   -1.660580

  5
PtNO3+ d(N-O)=2.55
   Pt        0.017155   -0.040836    0.304600
   O        -1.493881   -0.902990    0.485769
   O         1.517251   -0.902917    0.504354
   O         0.015489    1.715655    0.297465
   N        -0.056014    0.131088   -1.699166

  5
PtNO3+ d(N-O)=2.50
   Pt        0.008110   -0.048430    0.306344
   O        -1.496664   -0.910044    0.509884
   O         1.509720   -0.911995    0.499251
   O         0.007795    1.708913    0.270395
   N        -0.028961    0.161557   -1.692852

  5
PtNO3+ d(N-O)=2.45
   Pt        0.003873   -0.056205    0.306280
   O        -1.498457   -0.914142    0.526851
   O         1.504577   -0.922314    0.502119
   O         0.008261    1.700777    0.243904
   N        -0.018253    0.191884   -1.686132

  5
PtNO3+ d(N-O)=2.40
   Pt        0.001275   -0.061313    0.305848
   O        -1.494193   -0.929092    0.529359
   O         1.503912   -0.916415    0.527343
   O        -0.007378    1.694484    0.209061
   N        -0.003616    0.212337   -1.678590

  5
PtNO3+ d(N-O)=2.35
   Pt        0.000842   -0.069344    0.305793
   O        -1.493407   -0.934578    0.540913
   O         1.501662   -0.923952    0.536968
   O        -0.004205    1.685651    0.181903
   N        -0.004892    0.242223   -1.672556

  5
PtNO3+ d(N-O)=2.30
   Pt       -0.001827   -0.078912    0.304578
   O        -1.488033   -0.960352    0.525967
   O         1.502395   -0.921038    0.553995
   O        -0.023932    1.675537    0.170006
   N         0.011397    0.284764   -1.661524

  5
PtNO3+ d(N-O)=2.25
   Pt       -0.001804   -0.081914    0.305465
   O        -1.487055   -0.958697    0.547824
   O         1.499298   -0.922316    0.572933
   O        -0.020589    1.669165    0.123600
   N         0.010150    0.293762   -1.656800
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  5
PtNO3+ d(N-O)=2.20
   Pt       -0.002819   -0.088458    0.305692
   O        -1.483452   -0.971295    0.549288
   O         1.498669   -0.923417    0.587457
   O        -0.028163    1.660007    0.098636
   N         0.015766    0.323163   -1.648051

  5
PtNO3+ d(N-O)=2.15
   Pt       -0.003680   -0.091095    0.307600
   O        -1.481037   -0.975278    0.562734
   O         1.495769   -0.920636    0.611305
   O        -0.030998    1.652583    0.054568
   N         0.019946    0.334426   -1.643185

  5
PtNO3+ d(N-O)=2.10
   Pt       -0.005448   -0.098698    0.307253
   O        -1.478404   -0.988113    0.562720
   O         1.493536   -0.917990    0.635516
   O        -0.039572    1.643919    0.024278
   N         0.029888    0.360883   -1.636745

  5
PtNO3+ d(N-O)=2.12
   Pt       -0.052879   -0.060737    0.312425
   O        -1.423633   -1.133055    0.384080
   O         1.436721   -0.619395    1.012821
   O        -0.252267    1.621956   -0.174813
   N         0.292056    0.191231   -1.641489

  5
PtNO3+ d(N-O)=2.11
   Pt       -0.047579   -0.061040    0.313771
   O        -1.432701   -1.113347    0.405121
   O         1.442139   -0.640006    0.995724
   O        -0.235365    1.622581   -0.178325
   N         0.273504    0.191813   -1.643267

  5
PtNO3+ d(N-O)=2.10
   Pt       -0.043500   -0.072785    0.307408
   O        -1.436240   -1.110175    0.415597
   O         1.441651   -0.641981    0.999865
   O        -0.240226    1.620801   -0.184479
   N         0.278314    0.204141   -1.645366

  5
PtNO3+ d(N-O)=2.08
   Pt       -0.046831   -0.067521    0.311952
   O        -1.442712   -1.099023    0.433969
   O         1.441971   -0.657746    0.985200
   O        -0.218265    1.618139   -0.194766
   N         0.265836    0.206152   -1.643331

  5
PtNO3+ d(N-O)=2.07
   Pt       -0.057199   -0.122400    0.289725
   O        -1.402916   -1.196254    0.401288
   O         1.381736   -0.559946    1.137001
   O        -0.311117    1.596740   -0.248967
   N         0.389495    0.281860   -1.686024

  5
PtNO3+ d(N-O)=2.06
   Pt       -0.046450   -0.136931    0.285419
   O        -1.407509   -1.189362    0.409932
   O         1.413893   -0.630727    1.061569
   O        -0.281110    1.608666   -0.174903
   N         0.321174    0.348355   -1.688994

  5
PtNO3+ d(N-O)=2.05
   Pt       -0.022984   -0.140517    0.288503
   O        -1.452469   -1.070687    0.551222
   O         1.461560   -0.776229    0.896599
   O        -0.149746    1.628133   -0.131974
   N         0.163637    0.359300   -1.711326

  5
PtNO3+ d(N-O)=2.00
   Pt       -0.000113   -0.179886    0.270334
   O        -1.472525   -0.997692    0.639320
   O         1.473266   -0.997421    0.636704
   O        -0.000985    1.633753    0.010951
   N         0.000358    0.541246   -1.664288

  5
PtNO3+ d(N-O)=1.95
   Pt        0.008976   -0.200923    0.259184
   O        -1.469686   -0.976350    0.685968
   O         1.465472   -1.079607    0.531418
   O         0.058981    1.626712    0.044040
   N        -0.063744    0.630168   -1.627588

  5
PtNO3+ d(N-O)=1.90
   Pt       -0.008750   -0.217074    0.247176
   O        -1.471537   -1.082378    0.519375
   O         1.461839   -1.012509    0.657791
   O        -0.039338    1.626982    0.057929
   N         0.057786    0.684980   -1.589250

  5
PtNO3+ d(N-O)=1.85
   Pt       -0.008846   -0.238703    0.258896
   O        -1.487673   -1.082400    0.518626
   O         1.478490   -1.012585    0.658939
   O        -0.044859    1.624785    0.030161
   N         0.062888    0.708902   -1.573600

  5
PtNO3+ d(N-O)=1.75
   Pt       -0.077830   -0.104769   -0.089192
   O        -0.038208   -1.069394   -1.485311
   O         0.371542   -0.832399    1.441168
   O        -0.926813    1.574997   -0.067260
   N         0.794834    1.738352    0.200594

  5
PtNO3+ d(N-O)=1.70
   Pt       -0.088487   -0.098339   -0.096857
   O         0.037962   -1.046493   -1.499683
   O         0.118800   -0.881554    1.453678
   O        -0.797455    1.655825   -0.132597
   N         0.852704    1.677348    0.275458

  5
PtNO3+ d(N-O)=1.65
   Pt       -0.082113   -0.102603   -0.089390
   O         0.047728   -1.046392   -1.496133
   O         0.105122   -0.897223    1.453618
   O        -0.778933    1.667568   -0.112916
   N         0.831720    1.685438    0.244820

  5
PtNO3+ d(N-O)=1.60
   Pt       -0.063204   -0.104984   -0.001615
   O        -0.005652   -0.976929   -1.481126
   O         0.005500   -0.995818    1.465941
   O        -0.706392    1.708332    0.011606
   N         0.893272    1.676187    0.005192

  5
PtNO3+ d(N-O)=1.60
   Pt       -0.063307   -0.105015   -0.001599
   O        -0.005668   -0.976888   -1.481147
   O         0.005518   -0.995811    1.465970
   O        -0.706344    1.708210    0.011561
   N         0.893325    1.676291    0.005214

  5
PtNO3+ d(N-O)=1.55
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   Pt       -0.055927   -0.111464   -0.001783
   O        -0.007647   -0.983524   -1.480200
   O         0.003291   -1.002203    1.464914
   O        -0.682875    1.720191    0.011859
   N         0.866683    1.683785    0.005209

  5
PtNO3+ d(N-O)=1.50
   Pt       -0.046799   -0.118198   -0.001804
   O        -0.009416   -0.989813   -1.480012
   O         0.001501   -1.008613    1.464692
   O        -0.660504    1.735265    0.011829
   N         0.838741    1.688144    0.005295

  5
PtNO3+ d(N-O)=1.45
   Pt       -0.031887   -0.126236   -0.002095
   O        -0.013071   -0.997095   -1.480898
   O        -0.001648   -1.015579    1.465459
   O        -0.639298    1.753124    0.011484
   N         0.809427    1.692571    0.006051

  5
PtNO3+ d(N-O)=1.50
   Pt       -0.046427   -0.118131   -0.001802
   O        -0.009579   -0.989710   -1.480007
   O         0.001333   -1.008517    1.464691
   O        -0.660530    1.734970    0.011829
   N         0.838726    1.688173    0.005289

  5
PtNO3+ d(N-O)=1.45
   Pt       -0.032556   -0.126513   -0.002082
   O        -0.013025   -0.997367   -1.480820
   O        -0.001614   -1.015907    1.465399
   O        -0.639016    1.753267    0.011473
   N         0.809734    1.693306    0.006030

  5
PtNO3+ d(N-O)=1.40
   Pt       -0.007630   -0.135876   -0.002492
   O        -0.017834   -1.003234   -1.486155
   O        -0.006479   -1.021283    1.470588
   O        -0.620837    1.778211    0.011883
   N         0.776304    1.688967    0.006176

  5
PtNO3+ d(N-O)=1.30
   Pt       -0.069213   -0.182331    0.277717
   O        -0.170975   -0.778037   -1.386658
   O         0.206888   -1.367026    1.492662
   O        -0.441451    1.939605   -0.562310
   N         0.598274    1.694575    0.178589

  5
PtNO3+ d(N-O)=1.25
   Pt       -0.022813   -0.735051    0.045357
   O        -0.229715   -0.744772   -1.637427
   O         0.156552   -1.176105    1.672026
   O         0.092084    2.351663   -0.543154
   N         0.127416    1.611051    0.463198

  5
PtNO3+ d(N-O)=1.20
   Pt       -0.040385   -0.769942    0.081054
   O        -0.187924   -0.825803   -1.607173
   O         0.078221   -1.098858    1.739189
   O         0.114369    2.340164   -0.600758
   N         0.159242    1.661224    0.387689

  5
PtNO3+ d(N-O)=1.15
   Pt       -0.042891   -0.820373    0.077463
   O        -0.192618   -0.807122   -1.612869
   O         0.087386   -1.115296    1.742059
   O         0.118956    2.349033   -0.577886
   N         0.152690    1.700543    0.371231

  5
PtNO3+ d(N-O)=1.10
   Pt       -0.042738   -0.860064    0.083841
   O        -0.191763   -0.789996   -1.606074
   O         0.085421   -1.139444    1.751383
   O         0.120991    2.352964   -0.572124
   N         0.151613    1.743325    0.342974

5
PtNO3+ minimum C' d(N-O)=1.09
 Pt        0.028780  -0.434738 -0.044082
 O         0.216781  -1.073477 -1.669190
 O        -0.159874 -0.728738 1.603855
 O        -0.029806 2.449590  0.482417
 N         0.067645  1.694148  -0.373002

5
PtN2O2 minimum A d(N-N)=2.797
 Pt        -0.727892 0.263633  -0.161479
 O         -0.136100 1.076784  1.290191
 O         -0.161508 1.091315  -1.615075
 N         -0.158668 -1.355104 -0.174577
 N         -2.443795 0.257985  -0.146516

  5
PtN2O2 d(N-N)=2.77
   Pt       -0.724810    0.267982   -0.161485
   O        -0.133497    1.080439    1.290575
   O        -0.158948    1.095003   -1.615469
   N        -0.173928   -1.353098   -0.174407
   N        -2.436780    0.244286   -0.146670

  5
PtN2O2 d(N-N)=2.72
   Pt       -0.719728    0.275180   -0.161499
   O        -0.124189    1.085504    1.289888
   O        -0.159733    1.107309   -1.614699
   N        -0.200053   -1.349278   -0.180055
   N        -2.424261    0.215898   -0.141092

  5
PtN2O2 d(N-N)=2.67
   Pt       -0.714202    0.283032   -0.161520
   O        -0.099018    1.077603    1.290041
   O        -0.174046    1.127222   -1.614925
   N        -0.229837   -1.345583   -0.201853
   N        -2.410861    0.192338   -0.119198

  5
PtN2O2 d(N-N)=2.62
   Pt       -0.709418    0.289920   -0.161500
   O        -0.089636    1.081724    1.289395
   O        -0.174566    1.141041   -1.612631
   N        -0.256102   -1.341830   -0.208376
   N        -2.398242    0.163757   -0.114344

  5
PtN2O2 d(N-N)=2.57
   Pt       -0.619945    0.417382   -0.161637
   O        -0.149932    1.138665    1.379109
   O        -0.103410    1.102913   -1.703814
   N        -0.325563   -1.399982   -0.135351
   N        -2.429112    0.075633   -0.185763

  5
PtN2O2 d(N-N)=2.52
   Pt       -0.615392    0.423696   -0.161625
   O        -0.142659    1.142243    1.378972
   O        -0.101520    1.110266   -1.703639
   N        -0.353252   -1.394882   -0.139273
   N        -2.415141    0.053289   -0.181890

5
PtN2O2 minimum  d(N-N)=2.479
 Pt        -0.613084 0.426238  -0.161656
 O         -0.132657 1.148484  1.373746
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 O         -0.095775 1.119379  -1.698498
 N         -0.380524 -1.393911 -0.141545
 N         -2.405924 0.034422  -0.179504

  5
PtN2O2 d(N-N)=2.47
   Pt       -0.613097    0.426892   -0.161651
   O        -0.133413    1.152641    1.371980
   O        -0.094446    1.122117   -1.696738
   N        -0.383179   -1.393496   -0.140499
   N        -2.403829    0.026458   -0.180547

  5
PtN2O2 d(N-N)=2.42
   Pt       -0.608278    0.433188   -0.161647
   O        -0.126882    1.156499    1.372099
   O        -0.090131    1.127446   -1.696852
   N        -0.412601   -1.388510   -0.141946
   N        -2.390071    0.005990   -0.179111

  5
PtN2O2 d(N-N)=2.37
   Pt       -0.606047    0.436566   -0.161639
   O        -0.118599    1.163582    1.367851
   O        -0.087265    1.138457   -1.692567
   N        -0.439306   -1.384319   -0.144990
   N        -2.376746   -0.019674   -0.176112

  5
PtN2O2 d(N-N)=2.32
   Pt       -0.601917    0.442673   -0.161626
   O        -0.135400    1.184112    1.366627
   O        -0.063444    1.130540   -1.691284
   N        -0.465166   -1.378368   -0.126421
   N        -2.362036   -0.044346   -0.194752

  5
PtN2O2 d(N-N)=2.27
   Pt       -0.599719    0.444130   -0.161568
   O        -0.102057    1.175287    1.360929
   O        -0.075140    1.154025   -1.685098
   N        -0.499988   -1.376259   -0.148008
   N        -2.351058   -0.062570   -0.173712

  5
PtN2O2 d(N-N)=2.22
   Pt       -0.595406    0.450333   -0.161523
   O        -0.094834    1.176244    1.362069
   O        -0.076495    1.162321   -1.685563
   N        -0.525237   -1.369269   -0.153136
   N        -2.335992   -0.085016   -0.169303

  5
PtN2O2 d(N-N)=2.17
   Pt       -0.593476    0.452920   -0.161644
   O        -0.074824    1.175866    1.356015
   O        -0.083551    1.179696   -1.680420
   N        -0.553256   -1.364905   -0.163237
   N        -2.322857   -0.108964   -0.158170

  5
PtN2O2 d(N-N)=2.12
   Pt       -0.590148    0.457218   -0.161612
   O        -0.071251    1.181932    1.354581
   O        -0.079438    1.185366   -1.678975
   N        -0.579188   -1.358505   -0.163653
   N        -2.307938   -0.131398   -0.157798

  5
PtN2O2 d(N-N)=2.10
   Pt       -0.636147    0.540118   -0.165443
   O        -0.252534    1.331098    1.352192
   O        -0.091198    1.226485   -1.684888
   N        -0.420840   -1.407988   -0.088779
   N        -2.227244   -0.355102   -0.220540

  5
PtN2O2 d(N-N)=2.07
   Pt       -0.633338    0.545060   -0.165727
   O        -0.251783    1.336391    1.351469
   O        -0.088770    1.231307   -1.684368
   N        -0.435581   -1.411066   -0.090733
   N        -2.218491   -0.367079   -0.218099

  5
PtN2O2 d(N-N)=2.05
   Pt       -0.627856    0.547658   -0.161708
   O        -0.142470    1.280821    1.353788
   O        -0.176489    1.287033   -1.685085
   N        -0.463887   -1.416539   -0.169733
   N        -2.217261   -0.364361   -0.144721

  5
PtN2O2 d(N-N)=2.02
   Pt       -0.623607    0.549510   -0.161187
   O        -0.160078    1.289964    1.356762
   O        -0.155410    1.287018   -1.679212
   N        -0.478373   -1.415580   -0.158313
   N        -2.210495   -0.376301   -0.165508

  5
PtN2O2 d(N-N)=1.97
   Pt       -0.581157    0.532031   -0.161603
   O        -0.156176    1.301414    1.346553
   O        -0.149916    1.298396   -1.669517
   N        -0.509449   -1.377213   -0.159140
   N        -2.231265   -0.420015   -0.163751

  5
PtN2O2 d(N-N)=1.92
   Pt       -0.550068    0.515589   -0.161565
   O        -0.032788    1.234309    1.341282
   O        -0.046440    1.242929   -1.664906
   N        -0.714988   -1.382620   -0.166259
   N        -2.283679   -0.275595   -0.156009

  5
PtN2O2 d(N-N)=1.87
   Pt       -0.548611    0.517313   -0.161570
   O        -0.027889    1.241491    1.336059
   O        -0.041458    1.250066   -1.659689
   N        -0.741127   -1.376289   -0.166149
   N        -2.268878   -0.297969   -0.156107

  5
PtN2O2 d(N-N)=1.82
   Pt       -0.547581    0.518709   -0.161573
   O        -0.022580    1.249168    1.330184
   O        -0.036071    1.257693   -1.653818
   N        -0.767467   -1.370296   -0.166036
   N        -2.254265   -0.320661   -0.156214

  5
PtN2O2 d(N-N)=1.77
   Pt       -0.547824    0.519256   -0.161570
   O        -0.016055    1.258002    1.322507
   O        -0.029517    1.266511   -1.646149
   N        -0.794191   -1.364812   -0.165871
   N        -2.240377   -0.344345   -0.156373

  5
PtN2O2 d(N-N)=1.72
   Pt       -0.513915    0.485585   -0.161025
   O         0.079152    1.201153    1.309302
   O         0.185732    1.104405   -1.628387
   N        -1.072418   -1.325838   -0.121741
   N        -2.306515   -0.130694   -0.205604

  5
PtN2O2 d(N-N)=1.67
   Pt       -0.511662    0.488125   -0.161108
   O         0.086676    1.208641    1.304743
   O         0.193127    1.111837   -1.624007
   N        -1.099125   -1.317386   -0.122816
```

```
   N        -2.296978   -0.156604   -0.204267

  5
PtN2O2 d(N-N)=1.62
   Pt       -0.508485    0.491520   -0.161069
   O         0.095367    1.217438    1.300030
   O         0.201649    1.120733   -1.619215
   N        -1.127241   -1.310584   -0.124706
   N        -2.289253   -0.184495   -0.202496

  5
PtN2O2 d(N-N)=1.57
   Pt       -0.505253    0.494984   -0.161092
   O         0.108440    1.220547    1.296677
   O         0.204952    1.133446   -1.615773
   N        -1.154474   -1.302540   -0.129125
   N        -2.281628   -0.211825   -0.198143

  5
PtN2O2 d(N-N)=1.52
   Pt       -0.500596    0.498802   -0.161063
   O         0.117352    1.229765    1.293266
   O         0.213470    1.143063   -1.612353
   N        -1.183721   -1.296749   -0.130015
   N        -2.274467   -0.240270   -0.197290

  5
PtN2O2 d(N-N)=1.47
   Pt       -0.531764    0.533601   -0.163251
   O        -0.004231    1.349685    1.282238
   O         0.072339    1.278595   -1.617064
   N        -0.987778   -1.345208   -0.128478
   N        -2.176529   -0.482061   -0.180901

  5
PtN2O2 d(N-N)=1.42
   Pt       -0.545760    0.553165   -0.164240
   O        -0.089107    1.424014    1.275276
   O         0.032556    1.323522   -1.617210
   N        -0.912385   -1.360171   -0.113960
   N        -2.113267   -0.605917   -0.187324

  5
PtN2O2 d(N-N)=1.37
   Pt       -0.007089   -1.326989   -0.000324
   O         0.080499   -1.318279   -1.701091
   O        -0.094236   -1.311705    1.700427
   N        -0.577380    2.644870    0.217596
   N         0.721732    2.618889   -0.216607

  5
PtN2O2 d(N-N)=1.32
   Pt       -0.011460   -1.334191   -0.000147
   O         0.015359   -1.320578   -1.702928
   O        -0.024307   -1.318637    1.702779
   N        -0.586279    2.655430    0.045722
   N         0.730213    2.624762   -0.045425

  5
PtN2O2 d(N-N)=1.27
   Pt       -0.005815   -1.340428   -0.000119
   O        -0.049180   -1.326021   -1.702641
   O         0.034075   -1.326905    1.702496
   N        -0.552516    2.664311   -0.112661
   N         0.696963    2.635828    0.112927

  5
PtN2O2 d(N-N)=1.22
   Pt        0.000099   -1.346807    0.000068
   O        -0.012222   -1.331810   -1.702576
   O        -0.011043   -1.332061    1.702742
   N        -0.536596    2.666968   -0.001951
   N         0.683287    2.650495    0.001717

  5
PtN2O2 d(N-N)=1.17
   Pt       -0.004795   -1.367281    0.000048
   O        -0.004829   -1.354460   -1.702882
   O        -0.004990   -1.354616    1.702979
   N        -0.514371    2.734242    0.000247
   N         0.652512    2.648899   -0.000391

5
PtN2O2 minimum C" d(N-N)=1.095
   Pt       -0.020203   -1.395761   -0.000038
   O        -0.020032   -1.385544   -1.702960
   O        -0.020030   -1.385259    1.702882
   N        -0.455595    2.744540    0.000063
   N         0.639385    2.728808    0.000055

5
PtN2O2 minimum A d(N-O)=2.839
   Pt       -0.727892    0.263633   -0.161479
   O        -0.136100    1.076784    1.290191
   O        -0.161508    1.091315   -1.615075
   N        -0.158668   -1.355104   -0.174577
   N        -2.443795    0.257985   -0.146516

  5
PtN2O2 d(N-O)=2.80
   Pt       -0.732842    0.267997   -0.155051
   O        -0.136484    1.079288    1.295454
   O        -0.156094    1.070621   -1.612297
   N        -0.153679   -1.341959   -0.191222
   N        -2.448864    0.258665   -0.144340

  5
PtN2O2 d(N-O)=2.75
   Pt       -0.730787    0.286196   -0.146386
   O        -0.136709    1.100433    1.302405
   O        -0.141298    1.007221   -1.635135
   N        -0.159128   -1.335783   -0.195512
   N        -2.460042    0.276546   -0.132828

  5
PtN2O2 d(N-O)=2.70
   Pt       -0.736009    0.292047   -0.139046
   O        -0.143891    1.117762    1.303396
   O        -0.144698    0.973700   -1.641044
   N        -0.139000   -1.315745   -0.209816
   N        -2.464365    0.266848   -0.120946

  5
PtN2O2 d(N-O)=2.65
   Pt       -0.742063    0.297905   -0.131120
   O        -0.147830    1.121996    1.310736
   O        -0.136118    0.945738   -1.639226
   N        -0.132171   -1.301217   -0.234349
   N        -2.469781    0.270190   -0.113496

  5
PtN2O2 d(N-O)=2.60
   Pt       -0.747508    0.308997   -0.122032
   O        -0.148728    1.110711    1.329671
   O        -0.115546    0.916460   -1.636147
   N        -0.139363   -1.293033   -0.265901
   N        -2.476817    0.291478   -0.113048

  5
PtN2O2 d(N-O)=2.55
   Pt       -0.755173    0.332721   -0.110486
   O        -0.146075    1.102488    1.353965
   O        -0.119307    0.890141   -1.647430
   N        -0.120694   -1.277554   -0.304449
   N        -2.486714    0.286815   -0.099057

  5
PtN2O2 d(N-O)=2.50
   Pt       -0.779379    0.415002   -0.099308
   O        -0.152910    1.084604    1.413571
   O        -0.104440    0.824030   -1.696329
   N        -0.085983   -1.275782   -0.339697
   N        -2.505252    0.286757   -0.085693
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  5
PtN2O2 d(N-O)=2.45
   Pt       -0.940735    0.504353   -0.136975
   O        -0.134472    0.868266    1.432476
   O        -0.156962    0.693461   -1.748286
   N         0.228295   -1.215681   -0.261930
   N        -2.624090    0.484212   -0.092741

  5
PtN2O2 d(N-O)=2.40
   Pt       -0.940378    0.505668   -0.128040
   O        -0.137880    0.852456    1.446349
   O        -0.147374    0.689796   -1.734886
   N         0.222561   -1.202805   -0.306178
   N        -2.624892    0.489497   -0.084701

  5
PtN2O2 d(N-O)=2.35
   Pt       -0.941277    0.507216   -0.120291
   O        -0.146273    0.825209    1.464174
   O        -0.128906    0.678945   -1.718257
   N         0.214523   -1.196793   -0.344881
   N        -2.626030    0.520035   -0.088202

  5
PtN2O2 d(N-O)=2.30
   Pt       -0.943755    0.508331   -0.116880
   O        -0.154538    0.833018    1.467810
   O        -0.121862    0.646998   -1.713961
   N         0.220832   -1.181895   -0.362032
   N        -2.628640    0.528160   -0.082393

  5
PtN2O2 d(N-O)=2.25
   Pt       -0.940772    0.510100   -0.109696
   O        -0.153692    0.821874    1.478541
   O        -0.113759    0.631187   -1.706048
   N         0.206718   -1.172774   -0.400092
   N        -2.626458    0.544225   -0.070160

  5
PtN2O2 d(N-O)=2.20
   Pt       -0.942999    0.512046   -0.105058
   O        -0.158197    0.831623    1.481544
   O        -0.108729    0.599059   -1.699430
   N         0.211228   -1.158141   -0.414955
   N        -2.629266    0.550026   -0.069557

  5
PtN2O2 d(N-O)=2.20
   Pt       -0.949259    0.508049   -0.113039
   O        -0.162104    0.906805    1.454019
   O        -0.126891    0.553018   -1.716002
   N         0.245634   -1.145951   -0.368884
   N        -2.635342    0.512691   -0.063551

  5
PtN2O2 d(N-O)=2.15
   Pt       -0.942584    0.510624   -0.107463
   O        -0.167288    0.927403    1.460721
   O        -0.114887    0.530931   -1.708970
   N         0.228078   -1.135683   -0.394713
   N        -2.631282    0.501338   -0.057033

  5
PtN2O2 d(N-O)=2.10
   Pt       -0.004307    0.073889    0.049932
   O         1.176317   -0.840256   -0.962053
   O         0.956088    1.760353   -0.018523
   N        -0.871533   -0.832474    1.162035
   N        -1.133040    1.745270   -0.231393

  5
PtN2O2 d(N-O)=2.05
   Pt       -0.006290    0.064259    0.052310
   O         1.177409   -0.841775   -0.958951
   O         0.932780    1.772038   -0.026185
   N        -0.873260   -0.843109    1.161623
   N        -1.107114    1.755370   -0.228799

  5
PtN2O2 d(N-O)=2.00
   Pt       -0.014756    0.054189    0.050804
   O         1.140201   -0.857390   -0.986656
   O         0.929604    1.764748   -0.122163
   N        -0.861267   -0.842811    1.183763
   N        -1.070257    1.788047   -0.125750

  5
PtN2O2 d(N-O)=1.95
   Pt       -0.025401    0.044277    0.052713
   O         1.151157   -0.849769   -0.972333
   O         0.913119    1.773577   -0.159527
   N        -0.879521   -0.855992    1.178213
   N        -1.035829    1.794689   -0.099068

  5
PtN2O2 d(N-O)=1.95
   Pt        0.077411    0.046181    0.060797
   O        -0.546502   -0.870707   -1.354955
   O        -0.841373    1.718355   -0.460770
   N         0.506007   -0.851052    1.409058
   N         0.927982    1.864007    0.345870

  5
PtN2O2 d(N-O)=1.90
   Pt        0.097955    0.040825    0.076784
   O        -0.518125   -0.850065   -1.356889
   O        -0.829529    1.744853   -0.475597
   N         0.484380   -0.875310    1.427018
   N         0.888843    1.846480    0.328684

  5
PtN2O2 d(N-O)=1.85
   Pt        0.099526    0.035005    0.083338
   O        -0.503208   -0.848901   -1.360305
   O        -0.818291    1.755830   -0.449513
   N         0.472405   -0.886010    1.432562
   N         0.873093    1.850860    0.293917

  5
PtN2O2 d(N-O)=1.80
   Pt        0.101573    0.027192    0.090182
   O        -0.486161   -0.844768   -1.364898
   O        -0.810043    1.773397   -0.424151
   N         0.463645   -0.894211    1.441762
   N         0.854511    1.845174    0.257104

  5
PtN2O2 d(N-O)=1.75
   Pt        0.102076    0.019549    0.096597
   O        -0.433520   -0.845666   -1.380655
   O        -0.795175    1.782044   -0.416219
   N         0.425059   -0.898601    1.458684
   N         0.825085    1.849459    0.241592

  5
PtN2O2 d(N-O)=1.70
   Pt        0.102314    0.011265    0.101169
   O        -0.420320   -0.842946   -1.385405
   O        -0.780606    1.798236   -0.393898
   N         0.415087   -0.905765    1.466170
   N         0.807050    1.845993    0.211963

  5
PtN2O2 d(N-O)=1.65
   Pt        0.076363    0.001131    0.107407
   O        -0.319458   -0.812566   -1.439354
   O        -0.661038    1.844840   -0.438915
   N         0.206904   -0.940910    1.484612
   N         0.820753    1.814289    0.286249

  5
PtN2O2 d(N-O)=1.60
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   Pt        0.074796   -0.007661    0.112102
   O        -0.308337   -0.812632   -1.440870
   O        -0.646782    1.861732   -0.420432
   N         0.202843   -0.948614    1.490198
   N         0.801005    1.813959    0.259001

  5
PtN2O2 d(N-O)=1.55
   Pt        0.072644   -0.020038    0.119299
   O        -0.293715   -0.807720   -1.443944
   O        -0.635233    1.883605   -0.400373
   N         0.198789   -0.957272    1.500098
   N         0.781039    1.808210    0.224919

  5
PtN2O2 d(N-O)=1.50
   Pt        0.105487   -0.262561   -0.039284
   O        -0.153797   -1.056454   -1.574279
   O        -0.588043    2.375983    0.192585
   N         0.099803   -0.764709    1.563630
   N         0.660075    1.614526   -0.142653

  5
PtN2O2 d(N-O)=1.45
   Pt        0.035912   -0.314144   -0.091744
   O         0.217910   -1.202043   -1.589007
   O        -0.047601    2.547825    0.617325
   N        -0.163512   -0.713586    1.525984
   N         0.080816    1.588732   -0.462559

  5
PtN2O2 d(N-O)=1.40
   Pt        0.033676   -0.325291   -0.080930
   O         0.218876   -1.182348   -1.597006
   O        -0.044360    2.535151    0.586039
   N        -0.165983   -0.719130    1.538670
   N         0.081317    1.598401   -0.446774

  5
PtN2O2 d(N-O)=1.35
   Pt        0.033878   -0.337525   -0.069371
   O         0.216307   -1.147806   -1.613032
   O        -0.044126    2.522000    0.559180
   N        -0.158682   -0.737923    1.550304
   N         0.076148    1.608038   -0.427080

  5
PtN2O2 d(N-O)=1.30
   Pt        0.033433   -0.349010   -0.058207
   O         0.220722   -1.129660   -1.617376
   O        -0.043310    2.512909    0.527729
   N        -0.158140   -0.751253    1.561643
   N         0.070820    1.623798   -0.413789

  5
PtN2O2 d(N-O)=1.25
   Pt        0.033331   -0.367761   -0.053560
   O         0.221194   -1.113994   -1.630620
   O        -0.041730    2.488418    0.509092
   N        -0.157202   -0.737994    1.575642
   N         0.067932    1.638114   -0.400555

  5
PtN2O2 d(N-O)=1.20
   Pt        0.030425   -0.397288   -0.049389
   O         0.215188   -1.084429   -1.654392
   O        -0.032960    2.465392    0.500175
   N        -0.158013   -0.737775    1.587959
   N         0.068884    1.660885   -0.384354

  5
PtN2O2 d(N-O)=1.15
   Pt        0.029625   -0.433851   -0.044731
   O         0.216280   -1.075275   -1.668811
   O        -0.030523    2.450938    0.485071
   N        -0.159994   -0.728264    1.602850
   N         0.068137    1.693237   -0.374380

5
PtN2O2 minimum C' d(N-O)=1.145
   Pt        0.028787   -0.434737   -0.044090
   O         0.216785   -1.073475   -1.669199
   N        -0.159840   -0.728739    1.603850
   O        -0.029850    2.449589    0.482420
   N         0.067643    1.694146   -0.372982

5
PtN2O2 minimum A d(O-O)=2.905
   Pt       -0.727892    0.263633   -0.161479
   O        -0.136100    1.076784    1.290191
   O        -0.161508    1.091315   -1.615075
   N        -0.158668   -1.355104   -0.174577
   N        -2.443795    0.257985   -0.146516

  5
PtN2O2 d(O-O)=2.85
   Pt       -0.734554    0.254191   -0.161473
   O        -0.126494    1.090795    1.262465
   O        -0.151494    1.105105   -1.587390
   N        -0.164822   -1.364515   -0.174613
   N        -2.450599    0.249036   -0.146446

  5
PtN2O2 d(O-O)=2.80
   Pt       -0.739748    0.246800   -0.161466
   O        -0.122318    1.108206    1.237477
   O        -0.136599    1.114935   -1.562479
   N        -0.171694   -1.374414   -0.168277
   N        -2.457604    0.239085   -0.152710

  5
PtN2O2 d(O-O)=2.75
   Pt       -0.746323    0.237498   -0.161448
   O        -0.105500    1.113155    1.212269
   O        -0.137540    1.132182   -1.537478
   N        -0.177111   -1.380466   -0.179235
   N        -2.461489    0.232243   -0.141565

  5
PtN2O2 d(O-O)=2.70
   Pt       -0.752243    0.229147   -0.161425
   O        -0.086806    1.118432    1.186917
   O        -0.138519    1.151056   -1.512390
   N        -0.183527   -1.388452   -0.192053
   N        -2.466869    0.224430   -0.128505

  5
PtN2O2 d(O-O)=2.65
   Pt       -0.757706    0.221269   -0.161473
   O        -0.079078    1.130313    1.161993
   O        -0.129849    1.162806   -1.487321
   N        -0.189144   -1.396140   -0.191984
   N        -2.472186    0.216364   -0.128671

  5
PtN2O2 d(O-O)=2.60
   Pt       -0.763466    0.213361   -0.161427
   O        -0.072510    1.142444    1.137264
   O        -0.119773    1.173100   -1.462125
   N        -0.194401   -1.403843   -0.191543
   N        -2.477813    0.209550   -0.129625

  5
PtN2O2 d(O-O)=2.55
   Pt       -0.768908    0.205460   -0.161379
   O        -0.063689    1.153623    1.112019
   O        -0.112257    1.184556   -1.437331
   N        -0.199940   -1.411599   -0.190153
   N        -2.483169    0.202572   -0.130613

  5
PtN2O2 d(O-O)=2.50
   Pt       -0.032852    0.001393   -0.010998
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   O         0.884242   -1.014484    1.294632
   O        -0.588266    0.995444    1.499360
   N        -1.295602   -0.843985   -0.795903
   N         0.992439    0.861374   -1.076198

  5
PtN2O2 d(O-O)=2.45
   Pt       -0.033814    0.001483   -0.018390
   O         0.870881   -0.994556    1.308719
   O        -0.571875    0.975401    1.509283
   N        -1.295858   -0.842964   -0.804315
   N         0.990627    0.860377   -1.084405

  5
PtN2O2 d(O-O)=2.40
   Pt       -0.034548    0.001525   -0.024124
   O         0.857439   -0.974504    1.320710
   O        -0.555910    0.955226    1.517140
   N        -1.295765   -0.842476   -0.811505
   N         0.988746    0.859970   -1.091328

  5
PtN2O2 d(O-O)=2.35
   Pt       -0.035286    0.001548   -0.029966
   O         0.849988   -0.949834    1.333148
   O        -0.545840    0.930793    1.526549
   N        -1.290192   -0.848535   -0.820325
   N         0.981292    0.865769   -1.098512

  5
PtN2O2 d(O-O)=2.30
   Pt       -0.035943    0.001578   -0.035247
   O         0.833373   -0.932091    1.344850
   O        -0.526899    0.912936    1.533356
   N        -1.292592   -0.844536   -0.826699
   N         0.982023    0.861854   -1.105367

  5
PtN2O2 d(O-O)=2.25
   Pt       -0.036595    0.001616   -0.040622
   O         0.819620   -0.912307    1.357012
   O        -0.510590    0.892981    1.541346
   N        -1.292099   -0.843702   -0.834247
   N         0.979626    0.861153   -1.112596

  5
PtN2O2 d(O-O)=2.20
   Pt       -0.037210    0.001641   -0.045505
   O         0.807743   -0.890978    1.367619
   O        -0.496478    0.871514    1.548260
   N        -1.290160   -0.845478   -0.840929
   N         0.976068    0.863042   -1.118553

  5
PtN2O2 d(O-O)=2.15
   Pt       -0.037835    0.001667   -0.050490
   O         0.792147   -0.872463    1.378906
   O        -0.478581    0.852864    1.554964
   N        -1.288937   -0.846155   -0.847699
   N         0.973167    0.863828   -1.124787

  5
PtN2O2 d(O-O)=2.10
   Pt       -0.038549    0.001685   -0.055629
   O         0.773790   -0.855992    1.390524
   O        -0.457821    0.836331    1.561333
   N        -1.286194   -0.849082   -0.854694
   N         0.968735    0.866799   -1.130642

  5
PtN2O2 d(O-O)=2.05
   Pt       -0.040791    0.001956   -0.073185
   O         0.663624   -0.900296    1.426353
   O        -0.342208    0.880275    1.569079
   N        -1.239487   -0.915367   -0.874279
   N         0.918824    0.933173   -1.137074

  5
PtN2O2 d(O-O)=2.00
   Pt       -0.044187    0.002080   -0.099695
   O         0.581244   -0.917285    1.467582
   O        -0.252036    0.896840    1.588379
   N        -1.210290   -0.960983   -0.895705
   N         0.885231    0.979090   -1.149667

  5
PtN2O2 d(O-O)=1.95
   Pt       -0.045017    0.000433   -0.113311
   O         0.673388   -0.829278    1.480381
   O        -0.349896    0.825564    1.610335
   N        -1.057469   -1.112936   -0.922962
   N         0.738957    1.115958   -1.143550

  5
PtN2O2 d(O-O)=1.90
   Pt       -0.044489   -0.000216   -0.124703
   O         0.652500   -0.806820    1.499929
   O        -0.341685    0.808039    1.617502
   N        -1.055082   -1.115369   -0.933412
   N         0.748718    1.114107   -1.148423

  5
PtN2O2 d(O-O)=1.89
   Pt       -0.046402    0.000489   -0.126150
   O         0.683451   -0.788556    1.494149
   O        -0.356532    0.784068    1.626015
   N        -1.026216   -1.141287   -0.935566
   N         0.705662    1.145028   -1.147554

  5
PtN2O2 d(O-O)=1.88
   Pt       -0.046675    0.000417   -0.128342
   O         0.695316   -0.774538    1.494398
   O        -0.367857    0.770107    1.629071
   N        -1.002243   -1.160604   -0.939185
   N         0.681422    1.164360   -1.145049

  5
PtN2O2 d(O-O)=1.87
   Pt       -0.046789    0.000626   -0.129922
   O         0.682536   -0.777747    1.498978
   O        -0.354437    0.772838    1.630403
   N        -1.029567   -1.139500   -0.937752
   N         0.708221    1.143524   -1.150813

  5
PtN2O2 d(O-O)=1.85
   Pt       -0.047029    0.000476   -0.141919
   O         0.826553   -0.643017    1.503491
   O        -0.502832    0.632769    1.669644
   N        -1.137460   -1.030827   -0.946201
   N         0.820731    1.040341   -1.174122

  5
PtN2O2 d(O-O)=1.84
   Pt       -0.046483    0.000556   -0.142356
   O         0.824088   -0.638668    1.504869
   O        -0.500478    0.627863    1.669261
   N        -1.138004   -1.030161   -0.945883
   N         0.820841    1.040151   -1.174998

  5
PtN2O2 d(O-O)=1.87
   Pt       -0.043550   -0.000429   -0.131110
   O         0.992565   -0.393359    1.469885
   O        -0.688920    0.401578    1.663747
   N        -1.136021   -1.044671   -0.927054
   N         0.835888    1.036622   -1.164576

  5
PtN2O2 d(O-O)=1.87
   Pt       -0.045212   -0.001362   -0.132024
   O         0.986825   -0.402879    1.473683
   O        -0.680139    0.411982    1.661986
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   N        -1.127168   -1.054126   -0.930367
   N         0.825657    1.046126   -1.162386

  5
PtN2O2 d(O-O)=1.86
   Pt       -0.045503   -0.001010   -0.140909
   O         0.876494   -0.573036    1.504069
   O        -0.566642    0.580826    1.668346
   N        -1.034699   -1.122590   -0.954840
   N         0.730312    1.115551   -1.165774

  5
PtN2O2 d(O-O)=1.85
   Pt       -0.045636   -0.000988   -0.142055
   O         0.874579   -0.571389    1.503755
   O        -0.564840    0.579138    1.667651
   N        -1.035668   -1.123496   -0.953613
   N         0.731528    1.116476   -1.164846

  5
PtN2O2 d(O-O)=1.85
   Pt       -0.045656   -0.000986   -0.142075
   O         0.874518   -0.571526    1.504265
   O        -0.564650    0.579311    1.668187
   N        -1.035583   -1.123538   -0.954167
   N         0.731334    1.116481   -1.165317

  5
PtN2O2 d(O-O)=1.80
   Pt       -0.042656   -0.003246   -0.146415
   O         0.905397   -0.465231    1.515831
   O        -0.614309    0.486578    1.672526
   N        -0.895262   -1.222236   -0.974662
   N         0.606792    1.203876   -1.156387

  5
PtN2O2 d(O-O)=1.75
   Pt       -0.043091   -0.003226   -0.150704
   O         0.917646   -0.391347    1.521546
   O        -0.627686    0.414356    1.680578
   N        -0.796417   -1.278765   -0.989619
   N         0.509510    1.258723   -1.150908

  5
PtN2O2 d(O-O)=1.70
   Pt       -0.044282   -0.002813   -0.154206
   O         0.896287   -0.379695    1.529880
   O        -0.604924    0.402755    1.685247
   N        -0.795223   -1.278806   -0.994517
   N         0.508104    1.258300   -1.155510

  5
PtN2O2 d(O-O)=1.65
   Pt       -0.044549   -0.002722   -0.157848
   O         0.912515   -0.282254    1.534581
   O        -0.620898    0.305713    1.694069
   N        -0.647398   -1.344693   -1.014721
   N         0.360292    1.323696   -1.145188

  5
PtN2O2 d(O-O)=1.60
   Pt       -0.047430   -0.001924   -0.161995
   O         0.928175   -0.179339    1.533592
   O        -0.617099    0.197639    1.706849
   N        -0.488305   -1.394659   -1.036376
   N         0.184621    1.378024   -1.131176

  5
PtN2O2 d(O-O)=1.55
   Pt       -0.047616   -0.002278   -0.166479
   O         0.923525   -0.084492    1.539099
   O        -0.605223    0.101882    1.714297
   N        -0.325247   -1.424700   -1.059800
   N         0.014523    1.409330   -1.116225

  5
PtN2O2 d(O-O)=1.50
   Pt       -0.049588   -0.001984   -0.171036
   O         0.905781    0.031569    1.545679
   O        -0.583240   -0.014508    1.720882
   N        -0.111136   -1.434877   -1.088855
   N        -0.201854    1.419541   -1.095777

  5
PtN2O2 d(O-O)=1.45
   Pt        0.001400   -0.001896   -0.178273
   O         0.683875    0.005505    1.667006
   O        -0.765734    0.009508    1.633585
   N         0.016133   -1.434428   -1.098423
   N         0.024287    1.421052   -1.113003

5
PtN2O2 minimum C d(O-O)=1.405
   Pt        0.000208   -0.001921   -0.182996
   O         0.661135    0.005599    1.673782
   O        -0.743108    0.009498    1.642156
   N         0.016789   -1.435168   -1.103735
   N         0.024938    1.421732   -1.118314

 5
PtN3O- minimum A d(N-N)=2.868
   Pt        0.000000    0.000030    0.007665
   N        -1.433714   -0.827851    0.564351
   N         1.433715   -0.827851    0.564351
   N        -0.000001    1.655618    0.564267
   O        -0.000000    0.000055   -1.807610

  5
PtN3O- d(N-N)=2.85
   Pt       -0.002981   -0.001684    0.005156
   N        -1.436001   -0.829154    0.564234
   N         1.432409   -0.818438    0.566897
   N         0.007483    1.649777    0.566854
   O        -0.000911   -0.000500   -1.810117

  5
PtN3O- d(N-N)=2.80
   Pt       -0.008528   -0.004946   -0.000930
   N        -1.444787   -0.833991    0.548545
   N         1.426884   -0.795339    0.577102
   N         0.029193    1.630854    0.583827
   O        -0.002761    0.003423   -1.815520

  5
PtN3O- d(N-N)=2.75
   Pt       -0.015196   -0.008394   -0.007225
   N        -1.463725   -0.818597    0.538367
   N         1.410712   -0.773100    0.609280
   N         0.058119    1.621006    0.573913
   O         0.010091   -0.020914   -1.821310

  5
PtN3O- d(N-N)=2.70
   Pt       -0.021251   -0.011931   -0.013642
   N        -1.470427   -0.827021    0.524120
   N         1.406842   -0.750657    0.613856
   N         0.078203    1.599746    0.595933
   O         0.006633   -0.010135   -1.827244

  5
PtN3O- d(N-N)=2.65
   Pt       -0.027440   -0.015647   -0.020091
   N        -1.472363   -0.841695    0.512931
   N         1.407603   -0.725300    0.611972
   N         0.095048    1.576788    0.621500
   O        -0.002847    0.005855   -1.833288

  5
PtN3O- d(N-N)=2.60
   Pt       -0.033857   -0.019446   -0.025931
   N        -1.478563   -0.844863    0.508893
   N         1.403401   -0.699446    0.620023
   N         0.116492    1.559709    0.629089
   O        -0.007473    0.004048   -1.839051
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  5
PtN3O- d(N-N)=2.55
   Pt       -0.116659   -0.066164   -0.128558
   N        -1.521614   -0.869432    0.538537
   N         1.459794   -0.638315    0.703435
   N         0.196936    1.576997    0.712375
   O        -0.018457   -0.003084   -1.932764

  5
PtN3O- d(N-N)=2.50
   Pt       -0.119888   -0.067677   -0.134172
   N        -1.514138   -0.897879    0.523593
   N         1.461722   -0.605221    0.706021
   N         0.202612    1.554372    0.734324
   O        -0.030308    0.016406   -1.936742

  5
PtN3O- d(N-N)=2.45
   Pt       -0.123879   -0.070106   -0.138376
   N        -1.531399   -0.876281    0.521094
   N         1.449780   -0.585884    0.722299
   N         0.235547    1.542044    0.729956
   O        -0.030049   -0.009771   -1.941948

  5
PtN3O- d(N-N)=2.40
   Pt       -0.126800   -0.072674   -0.143425
   N        -1.531640   -0.887423    0.512454
   N         1.446656   -0.554258    0.730353
   N         0.247375    1.524594    0.740196
   O        -0.035591   -0.010238   -1.946553

  5
PtN3O- d(N-N)=2.35
   Pt       -0.129995   -0.076038   -0.146944
   N        -1.521902   -0.909755    0.512918
   N         1.452514   -0.509708    0.730249
   N         0.251555    1.510171    0.747249
   O        -0.052172   -0.014669   -1.950448

  5
PtN3O- d(N-N)=2.30
   Pt       -0.138673   -0.082000   -0.167699
   N        -1.530003   -0.950746    0.520339
   N         1.469848   -0.466729    0.734024
   N         0.269261    1.494505    0.780405
   O        -0.070432    0.004970   -1.974045

  5
PtN3O- d(N-N)=2.25
   Pt       -0.142523   -0.084062   -0.171635
   N        -1.528425   -0.962815    0.512461
   N         1.467395   -0.437367    0.736839
   N         0.283638    1.475250    0.792657
   O        -0.080084    0.008995   -1.977298

  5
PtN3O- d(N-N)=2.20
   Pt       -0.145228   -0.088342   -0.176170
   N        -1.540624   -0.950674    0.505854
   N         1.452417   -0.404543    0.765750
   N         0.300946    1.470003    0.779554
   O        -0.067509   -0.026444   -1.981964

  5
PtN3O- d(N-N)=2.10
   Pt       -0.155427   -0.091874   -0.180930
   N        -1.556530   -0.931618    0.517376
   N         1.440862   -0.366554    0.767546
   N         0.364794    1.436780    0.775658
   O        -0.093698   -0.046733   -1.986627

  5
PtN3O- d(N-N)=2.05
   Pt       -0.190543   -0.112854   -0.188141
   N        -1.567611   -0.917401    0.483544
   N         1.451719   -0.333015    0.794742
   N         0.414635    1.435286    0.786585
   O        -0.108201   -0.072015   -1.983707

  5
PtN3O- d(N-N)=2.00
   Pt       -0.203628   -0.122451   -0.196429
   N        -1.580837   -0.925067    0.471481
   N         1.457494   -0.300037    0.809184
   N         0.446613    1.425668    0.801267
   O        -0.119642   -0.078113   -1.992479

  5
PtN3O- d(N-N)=2.00
   Pt       -0.204509   -0.121176   -0.196285
   N        -1.409489   -1.176675    0.453788
   N         1.561563   -0.252112    0.597601
   N         0.391391    1.320844    0.993211
   O        -0.338956    0.229121   -1.955289

  5
PtN3O- d(N-N)=1.95
   Pt       -0.198371   -0.134685   -0.200722
   N        -1.445249   -1.132404    0.459790
   N         1.505430   -0.153501    0.746616
   N         0.332558    1.398728    0.878746
   O        -0.194369    0.021864   -1.991404

  5
PtN3O- d(N-N)=1.90
   Pt       -0.204538   -0.132277   -0.203656
   N        -1.368408   -1.236358    0.440184
   N         1.541283   -0.112150    0.665180
   N         0.340020    1.328628    0.967055
   O        -0.308357    0.152159   -1.975739

  5
PtN3O- d(N-N)=1.90
   Pt       -0.213011   -0.122266   -0.200783
   N        -1.578831   -0.934613    0.477805
   N         1.455833   -0.252183    0.801924
   N         0.491742    1.385024    0.811063
   O        -0.155732   -0.075961   -1.996983

  5
PtN3O- d(N-N)=1.85
   Pt       -0.215936   -0.122586   -0.205356
   N        -1.504978   -1.057231    0.466500
   N         1.495501   -0.213618    0.717688
   N         0.483516    1.323574    0.905911
   O        -0.258103    0.069863   -1.991717

  5
PtN3O- d(N-N)=1.80
   Pt       -0.219466   -0.122812   -0.208471
   N        -1.508627   -1.057490    0.461631
   N         1.490250   -0.189115    0.726132
   N         0.501751    1.304071    0.908524
   O        -0.263908    0.065347   -1.994790

  5
PtN3O- d(N-N)=1.75
   Pt       -0.221695   -0.125155   -0.212151
   N        -1.511490   -1.058678    0.456849
   N         1.484271   -0.165288    0.737595
   N         0.520417    1.285312    0.908609
   O        -0.271504    0.063810   -1.997877

  5
PtN3O- d(N-N)=1.70
   Pt       -0.225920   -0.126682   -0.213214
   N        -1.515827   -1.061478    0.450706
   N         1.474453   -0.140759    0.740730
   N         0.541954    1.270044    0.914163
   O        -0.274660    0.058876   -1.999359

  5
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PtN3O- d(N-N)=1.65
   Pt       -0.226041   -0.130389   -0.194155
   N        -1.607222   -0.927027    0.437306
   N         1.419130   -0.133592    0.821064
   N         0.593950    1.295246    0.821227
   O        -0.179817   -0.104236   -1.992417

  5
PtN3O- d(N-N)=1.60
   Pt       -0.229406   -0.134264   -0.219628
   N        -1.688261   -0.774815    0.437775
   N         1.360009   -0.124892    0.920324
   N         0.660670    1.305339    0.761061
   O        -0.103012   -0.271367   -2.006508

  5
PtN3O- d(N-N)=1.55
   Pt       -0.232591   -0.134992   -0.222512
   N        -1.690843   -0.780063    0.430665
   N         1.356963   -0.100335    0.922099
   N         0.679484    1.285873    0.773947
   O        -0.113014   -0.270483   -2.011174

  5
PtN3O- d(N-N)=1.50
   Pt       -0.238007   -0.136119   -0.203266
   N        -1.706147   -0.790116    0.402704
   N         1.361581   -0.070618    0.918764
   N         0.704820    1.270222    0.774498
   O        -0.122247   -0.273369   -1.999676

  5
PtN3O- d(N-N)=1.45
   Pt       -0.262412   -0.098744   -0.223148
   N        -1.760145   -0.671743    0.402134
   N         1.375676   -0.256309    0.866573
   N         0.859405    1.098656    0.872409
   O        -0.212525   -0.071859   -2.024943

  5
PtN3O- d(N-N)=1.40
   Pt       -0.268778   -0.101563   -0.210704
   N        -1.778871   -0.678590    0.377481
   N         1.384506   -0.226359    0.871324
   N         0.886850    1.082197    0.875965
   O        -0.223707   -0.075684   -2.021043

  5
PtN3O- d(N-N)=1.35
   Pt       -0.275755   -0.103967   -0.221405
   N        -1.785583   -0.681485    0.374080
   N         1.388103   -0.197955    0.883879
   N         0.907702    1.063663    0.889847
   O        -0.234467   -0.080255   -2.033376

  5
PtN3O- d(N-N)=1.30
   Pt       -0.288822   -0.109046   -0.216409
   N        -1.808553   -0.688454    0.358061
   N         1.399949   -0.167228    0.890747
   N         0.938061    1.047940    0.895736
   O        -0.240637   -0.083211   -2.035110

  5
PtN3O- d(N-N)=1.25
   Pt       -0.298864   -0.113130   -0.224210
   N        -1.822301   -0.693394    0.350300
   N         1.408939   -0.137106    0.904791
   N         0.964238    1.031105    0.909758
   O        -0.252013   -0.087473   -2.047614

  5
PtN3O- d(N-N)=1.20
   Pt       -0.318310   -0.119926   -0.224522
   N        -1.849181   -0.703968    0.336286
   N         1.425625   -0.104130    0.915110
   N         0.998885    1.017419    0.919689
   O        -0.257020   -0.089394   -2.053539

  5
PtN3O- d(N-N)=1.15
   Pt       -1.428122   -0.548645   -0.636660
   N        -2.834890   -1.081912    0.163649
   N         2.317368    0.277689    0.868051
   N         1.894622    1.344179    0.947966
   O         0.051022    0.008690   -1.449981

  5
PtN3O- d(N-N)=1.10
   Pt       -1.438791   -0.553184   -0.636651
   N        -2.851467   -1.088937    0.151332
   N         2.326458    0.307016    0.875237
   N         1.920860    1.327057    0.945991
   O         0.042940    0.008050   -1.442884

5
PtN3O- minimum C" d(N-N)=1.095
   Pt       -0.240458    1.426681    0.000922
   N        -1.655077    2.376872    0.005784
   N         0.340581   -2.654389   -0.548775
   N         0.342159   -2.654862    0.546183
   O         1.226389    0.422137   -0.004114

5
PtN3O- minimum A d(N-O)=2.893
   Pt        0.000000    0.000030    0.007665
   N        -1.433714   -0.827851    0.564351
   N         1.433715   -0.827851    0.564351
   N        -0.000001    1.655618    0.564267
   O        -0.000000    0.000055   -1.807610

  5
PtN3O- d(N-O)=2.85
   Pt       -0.000020   -0.007146    0.011972
   N        -1.433820   -0.834086    0.569428
   N         1.433805   -0.834097    0.569347
   N        -0.000019    1.653012    0.539827
   O         0.000054    0.022317   -1.797550

  5
PtN3O- d(N-O)=2.80
   Pt        0.000135   -0.015592    0.016864
   N        -1.433855   -0.835656    0.583788
   N         1.434224   -0.844827    0.570041
   N         0.007805    1.650940    0.508023
   O        -0.008309    0.045136   -1.785693

  5
PtN3O- d(N-O)=2.75
   Pt        0.000075   -0.023197    0.022317
   N        -1.435159   -0.835446    0.597076
   N         1.433527   -0.844890    0.588062
   N         0.006867    1.653551    0.459803
   O        -0.005310    0.049983   -1.774234

  5
PtN3O- d(N-O)=2.70
   Pt       -0.000082   -0.031667    0.027785
   N        -1.435696   -0.846842    0.597016
   N         1.433762   -0.848594    0.598896
   N         0.000686    1.649349    0.432399
   O         0.001329    0.077755   -1.763072

  5
PtN3O- d(N-O)=2.65
   Pt       -0.000197   -0.038841    0.033756
   N        -1.435806   -0.856690    0.598924
   N         1.434530   -0.842272    0.621609
   N        -0.011465    1.649179    0.390182
   O         0.012937    0.088624   -1.751447

  5
PtN3O- d(N-O)=2.60
   Pt       -0.000237   -0.048927    0.039277
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   N        -1.435994   -0.865619    0.605114
   N         1.436265   -0.848138    0.628361
   N        -0.011936    1.645592    0.361697
   O         0.011902    0.117093   -1.741425

  5
PtN3O- d(N-O)=2.55
   Pt       -0.000010   -0.084730    0.038147
   N        -1.442781   -0.884476    0.613585
   N         1.442973   -0.844524    0.664453
   N        -0.029877    1.653054    0.321832
   O         0.029695    0.160678   -1.744993

  5
PtN3O- d(N-O)=2.50
   Pt        0.027956   -0.205304    0.029645
   N        -1.481638   -0.943014    0.551725
   N         1.459237   -0.854119    0.785374
   N         0.041948    1.711615    0.290678
   O        -0.047502    0.290822   -1.764400

  5
PtN3O- d(N-O)=2.45
   Pt        0.030256   -0.210270    0.042292
   N        -1.482438   -0.946374    0.552725
   N         1.452486   -0.846796    0.818683
   N         0.047385    1.716556    0.233328
   O        -0.047688    0.286884   -1.754007

  5
PtN3O- d(N-O)=2.40
   Pt        0.032091   -0.218913    0.052334
   N        -1.480165   -0.963394    0.548199
   N         1.453856   -0.840356    0.835565
   N         0.052310    1.718122    0.196656
   O        -0.058092    0.304540   -1.739731

  5
PtN3O- d(N-O)=2.35
   Pt        0.028304   -0.229871    0.060974
   N        -1.482630   -0.977399    0.543764
   N         1.455804   -0.838443    0.845068
   N         0.065434    1.716188    0.167937
   O        -0.066911    0.329525   -1.724721

  5
PtN3O- d(N-O)=2.30
   Pt        0.023501   -0.240502    0.072538
   N        -1.486693   -0.988376    0.541601
   N         1.459221   -0.840013    0.846411
   N         0.071440    1.717448    0.138833
   O        -0.067468    0.351444   -1.706361

  5
PtN3O- d(N-O)=2.25
   Pt        0.021400   -0.251817    0.084206
   N        -1.481233   -1.012047    0.540028
   N         1.473118   -0.830010    0.842482
   N         0.055639    1.715795    0.115581
   O        -0.068923    0.378079   -1.689274

  5
PtN3O- d(N-O)=2.20
   Pt        0.016360   -0.261607    0.095696
   N        -1.485668   -1.015910    0.544984
   N         1.477569   -0.835838    0.836195
   N         0.049107    1.714545    0.088060
   O        -0.057367    0.398810   -1.671913

  5
PtN3O- d(N-O)=2.15
   Pt        0.010208   -0.271269    0.107542
   N        -1.491672   -1.001746    0.577768
   N         1.486408   -0.854414    0.807598
   N         0.051815    1.712375    0.055580
   O        -0.056757    0.415054   -1.655465

  5
PtN3O- d(N-O)=2.10
   Pt        0.006333   -0.280198    0.115058
   N        -1.495786   -1.000589    0.589907
   N         1.489907   -0.862973    0.798345
   N         0.036729    1.706983    0.030187
   O        -0.037182    0.436777   -1.640475

  5
PtN3O- d(N-O)=2.05
   Pt        0.002167   -0.244348    0.144017
   N        -1.441383   -1.139071    0.475034
   N         1.440331   -0.812393    0.920571
   N        -0.192937    1.631821    0.030251
   O         0.191823    0.563990   -1.676851

  5
PtN3O- d(N-O)=2.00
   Pt        0.000357   -0.237053    0.166366
   N        -1.464068   -1.003111    0.672617
   N         1.464138   -0.902023    0.801026
   N        -0.054781    1.634928   -0.049410
   O         0.054355    0.507259   -1.697577

  5
PtN3O- d(N-O)=2.00
   Pt        0.000827   -0.238013    0.164819
   N        -1.464110   -1.002879    0.672518
   N         1.464267   -0.901512    0.802622
   N        -0.053965    1.634600   -0.049015
   O         0.052982    0.507804   -1.697922

  5
PtN3O- d(N-O)=1.95
   Pt       -0.000368   -0.222902    0.190420
   N        -1.467172   -0.873452    0.832561
   N         1.463870   -0.862574    0.849136
   N        -0.004634    1.614260   -0.249536
   O         0.008305    0.344668   -1.729559

  5
PtN3O- d(N-O)=1.90
   Pt       -0.000078   -0.255534    0.159505
   N        -1.464939   -0.977459    0.725319
   N         1.463592   -0.966910    0.741534
   N        -0.005583    1.621615   -0.072736
   O         0.007009    0.578289   -1.660599

  5
PtN3O- d(N-O)=1.90
   Pt        0.000421   -0.250957    0.165993
   N        -1.463519   -1.005351    0.690377
   N         1.460026   -0.898383    0.827453
   N        -0.054939    1.618598   -0.116709
   O         0.058011    0.536096   -1.674089

  5
PtN3O- d(N-O)=1.85
   Pt        0.000766   -0.258194    0.164547
   N        -1.462844   -1.008553    0.696015
   N         1.459075   -0.901662    0.833056
   N        -0.053466    1.610122   -0.141340
   O         0.056469    0.558290   -1.659254

  5
PtN3O- d(N-O)=1.80
   Pt        0.002619   -0.283836    0.132516
   N        -1.455146   -1.079968    0.611706
   N         1.467305   -1.002300    0.704562
   N        -0.044053    1.608734    0.014239
   O         0.029275    0.757373   -1.569998

  5
PtN3O- d(N-O)=1.75
   Pt        0.002903   -0.290839    0.130866
   N        -1.454402   -1.084148    0.617213
   N         1.466416   -1.006470    0.710178
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   N        -0.042963    1.602640   -0.011452
   O         0.028046    0.778820   -1.553781

  5
PtN3O- d(N-O)=1.70
   Pt        0.003096   -0.296480    0.129382
   N        -1.453129   -1.088659    0.622364
   N         1.465061   -1.011068    0.715202
   N        -0.042032    1.597126   -0.037234
   O         0.027004    0.799085   -1.536689

  5
PtN3O- d(N-O)=1.65
   Pt        0.003386   -0.304513    0.127102
   N        -1.453582   -1.091589    0.628013
   N         1.465311   -1.013984    0.720880
   N        -0.041026    1.589062   -0.062078
   O         0.025911    0.821028   -1.520894

  5
PtN3O- d(N-O)=1.60
   Pt        0.003688   -0.311860    0.123858
   N        -1.450344   -1.106151    0.640361
   N         1.462068   -1.028715    0.733017
   N        -0.040158    1.595445   -0.094644
   O         0.024745    0.851283   -1.509568

  5
PtN3O- d(N-O)=1.55
   Pt        0.004013   -0.320515    0.121086
   N        -1.448755   -1.119067    0.651649
   N         1.460463   -1.041724    0.744246
   N        -0.039264    1.600715   -0.126416
   O         0.023544    0.880594   -1.497541

  5
PtN3O- d(N-O)=1.50
   Pt        0.000255   -0.320549    0.139577
   N        -1.455906   -1.057923    0.760317
   N         1.454749   -1.047389    0.776457
   N        -0.004513    1.599128   -0.248760
   O         0.005415    0.826732   -1.534569

  5
PtN3O- d(N-O)=1.45
   Pt        0.131493   -0.405085    0.331723
   N        -1.491710   -1.053921    0.542157
   N         1.578553   -1.088180    0.985418
   N         0.202183    1.486142   -0.363858
   O        -0.420520    1.061043   -1.602418

  5
PtN3O- d(N-O)=1.40
   Pt        0.086594   -0.477824    0.397951
   N        -1.464449   -1.207064    0.564126
   N         1.547376   -0.955772    1.198248
   N         0.434327    1.039770   -0.757041
   O        -0.603847    1.600889   -1.510262

  5
PtN3O- d(N-O)=1.35
   Pt        0.081986   -0.487634    0.397914
   N        -1.474368   -1.207529    0.565827
   N         1.559847   -0.955807    1.176773
   N         0.412494    1.045260   -0.762002
   O        -0.579958    1.605709   -1.485490

  5
PtN3O- d(N-O)=1.30
   Pt        0.107425   -0.484666    0.408018
   N        -1.402469   -1.292457    0.611235
   N         1.635903   -0.830832    1.155235
   N         0.322934    1.062419   -0.793254
   O        -0.663793    1.545536   -1.488212

  5
PtN3O- d(N-O)=1.25
   Pt        0.099916   -0.466898    0.439663
   N        -1.360372   -1.379237    0.550849
   N         1.592741   -0.646013    1.310385
   N         0.291780    1.060506   -0.821189
   O        -0.624066    1.431641   -1.586686

5
PtN3O- minimum C' d(N-O)=1.201
 Pt        0.054938  -0.505458 0.427454
 N        -1.481588 -1.292015 0.487967
 N         1.543564  -0.814377 1.271423
 N         0.365836  1.077621  -0.788468
 O        -0.482751 1.534226  -1.505353
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