Electronic Supplementary Information

On the Electronic Structure and Conflicting d-Orbital Aromaticity in the $Re_3O_3^-$ Cluster

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Molecular Orbital Analyses for the high-lying $Re_3O_3^-$ D_{3h} structures.

Figures S1-S2. Alternative optimized structures for $Re_3O_3^-$ and Re_3O_3 at the B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ level.

Figure S3. Molecular orbital pictures for the $Re_3O_3^-$ D_{3h} ($^3A_1'$) structure, which lies 3.06 eV above the global minimum at B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ level.

Figure S4. Molecular orbital pictures for the $Re_3O_3^-$ D_{3h} ($^1A_1'$) structure, which lies 5.36 eV above the global minimum at B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ level.

Table S1. Cartesian coordinates for all optimized structures for $Re_3O_3^-$ and Re_3O_3 at B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ level.

Molecular Orbital Analyses for the High-Lying $Re_3O_3^-$ D_{3h} Structures

The highly symmetric $Re_3O_3^-$ D_{3h} ($^3A_1'$) and D_{3h} ($^1A_1'$) structures (Figures S3 and S4) seem to be tempting candidates to account for the vibrationally-resolved photoelectron spectrum (Figure 1a), which hints relatively high symmetry for both the anion and neutral clusters. This hypothesis turns out to be wrong, in terms of both their energetics and their simulated PES spectra (Figure 3d and 3e). Thus a critical question arises: Why are these D_{3h} structures so much higher in energy relative to the C_{2v} ($^1A_1$) global minimum (Figure 2a)?

A three-center transition metal system in principle is capable of forming four completely bonding (two σ-, one π-, and one δ-) MOs.[S1,S2] Ideally all these MOs need to be filled in order for a $Re_3O_3^-$ structure to be stable. However, the D_{3h} structures each possess only three completely bonding MOs, and the two additional electrons that are supposed to occupy the missing σ-MO are forced to occupy the antibonding MOs instead.

To be specific, HOMO−5 ($1a_1'$) and HOMO−1 ($1e'$) of the D_{3h} ($^3A_1'$) structure (Figure S3) represent the σ/σ* combination and HOMO−2 ($1a_2''$) and HOMO−3 ($1e''$) represent the π/π* combination. These MOs can be roughly localized as three (albeit weak) Re=Re double bonds. The remaining HOMO−4 ($2a_1'$) and half-occupied HOMO ($2e'$) collectively render δ aromaticity for this species, according to the reversed $4n$ Hückel aromaticity rule for triplet coupled electrons. Overall, the Re-Re bonding (2.424 Å) in D_{3h} ($^3A_1'$) is slightly weaker than typical Re=Re double bonds (2.38 Å).[S3]

For the D_{3h} ($^1A_1'$) structure (Figure S4), the HOMO−5 ($1a_1'$) and HOMO−2 ($1e'$) form the σ framework and may be considered as three Re-Re σ-bonds, which are largely canceled by the net antibonding nature of the π framework: HOMO−4 ($1a_2''$), HOMO−1 ($1e''$), and HOMO ($1a_1''$). The remaining completely bonding HOMO−3 ($2a_1'$) renders δ-aromaticity to this species. Not surprisingly, the net Re-Re bonding (2.699 Å) in D_{3h} ($^1A_1'$) is even weaker than typical Re-Re single bonds (2.62 Å),[S3] commensurate with its energetic instability.

In contrast to these high-lying D_{3h} structures, all four bonding MOs are fully occupied in the C_{2v} ($^1A_1$) global minimum, and in addition the structural distortion to C_{2v} poses extra

stabilization to the corresponding σ* and π* MOs.

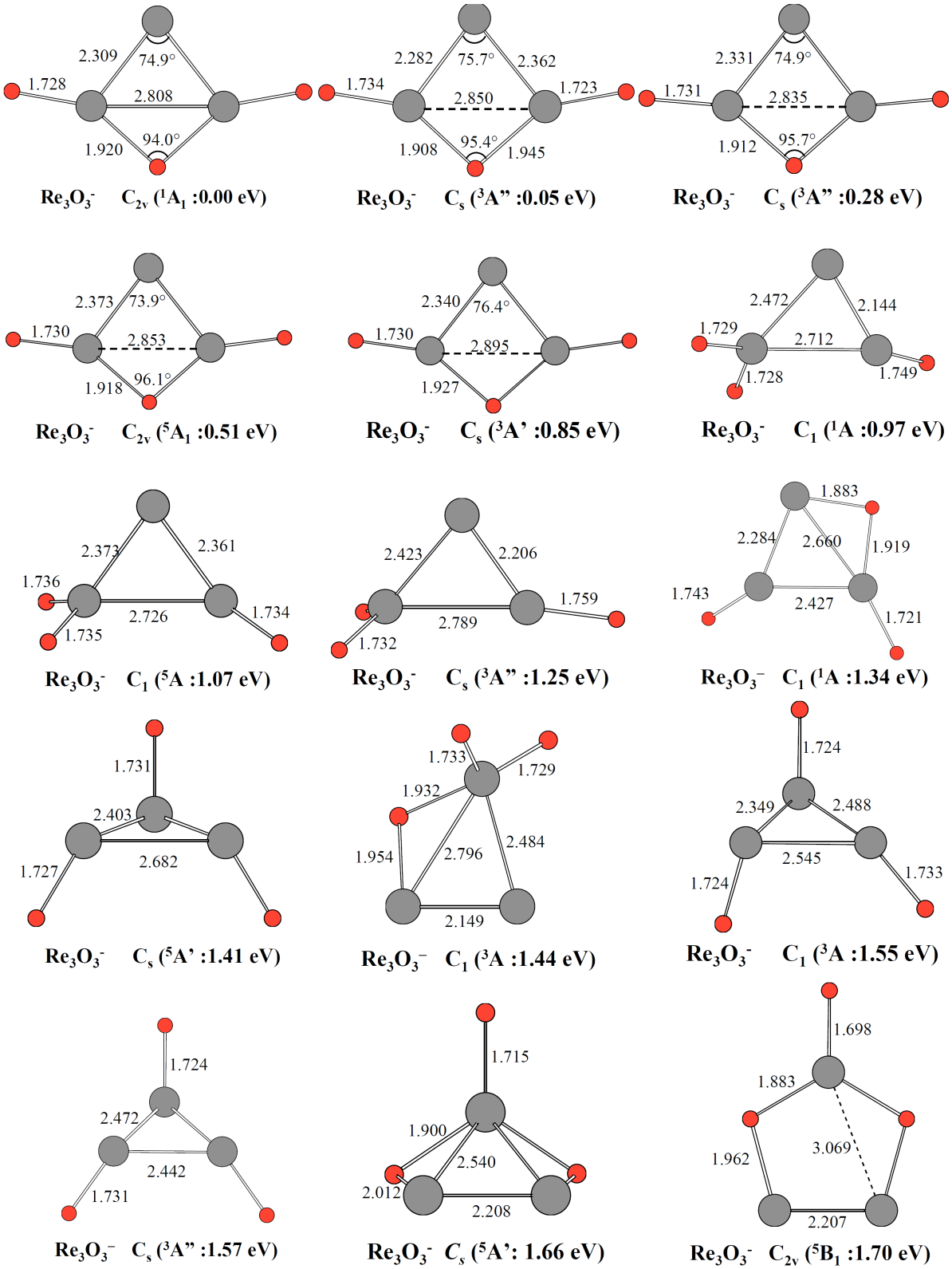
References:

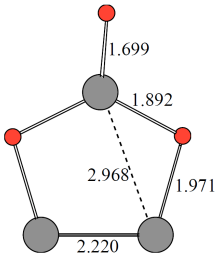
(S1) Averkiev, B. B.; Boldyrev, A. I. Hf_3 Cluster Is Triply (σ-, π-, and δ-) Aromatic in the Lowest D_{3h}, $^1A_1'$ State. *J. Phys. Chem. A* **2007**, *111*, 12864–12866.

(S2) Zhai, H. J.; Wang, B.; Huang, X.; Wang, L. S. Structural Evolution, Sequential Oxidation, and Chemical Bonding in Tritantalum Oxide Clusters: $Ta_3O_n^-$ and Ta_3O_n (n = 1–8). *J. Phys. Chem. A* **2009**, *113*, 9804–9813.

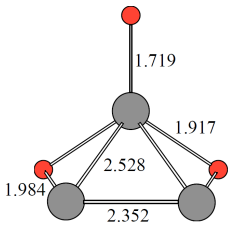
(S3) Pyykkö, P.; Atsumi, M. Molecular Double-Bond Covalent Radii for Elements Li–E112. *Chem. Eur. J.* **2009**, *15*, 12770–12779.

Figure S1. Optimized structures (distances in angstroms and angles in degrees) and their relative energies for $Re_3O_3^-$ cluster.

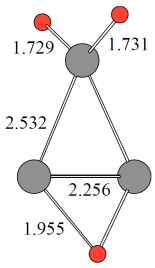




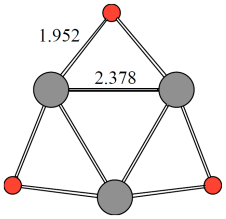
$Re_3O_3^-$ C_s ($^7A'$:1.79 eV)



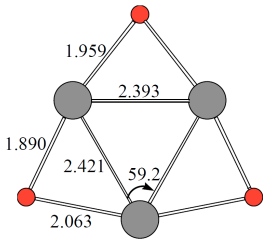
$Re_3O_3^-$ C_s ($^7A''$:1.96 eV)



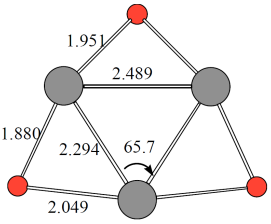
$Re_3O_3^-$ C_1 (^3A :2.05 eV)



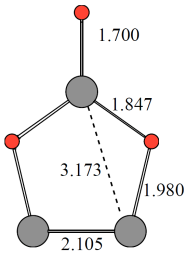
$Re_3O_3^-$ C_{3v} ($^3A_1$:2.08 eV)



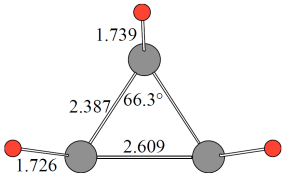
$Re_3O_3^-$ C_s ($^5A'$:2.19 eV)



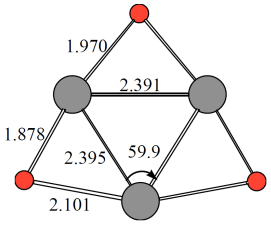
$Re_3O_3^-$ C_s ($^1A'$:2.27 eV)



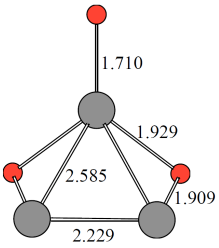
$Re_3O_3^-$ C_{2v} ($^3B_2$:2.31 eV)



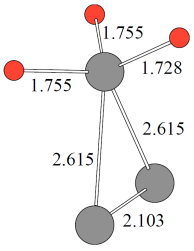
$Re_3O_3^-$ C_s ($^5A''$:2.35 eV)



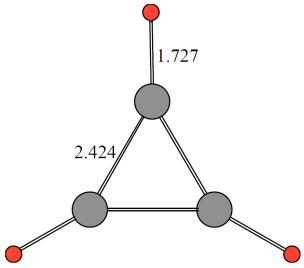
$Re_3O_3^-$ C_{2v} ($^5A_1$:2.35 eV)



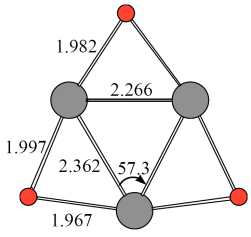
$Re_3O_3^-$ C_s ($^1A'$:2.45 eV)



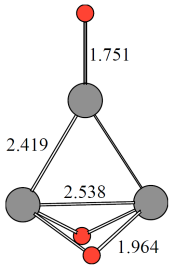
$Re_3O_3^-$ C_s ($^1A'$:2.49 eV)



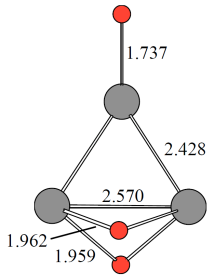
$Re_3O_3^-$ D_{3h} ($^3A_1'$:3.06 eV)



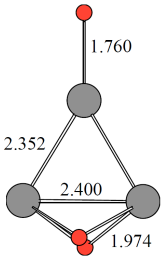
$Re_3O_3^-$ C_{2v} ($^1A_1$:3.28 eV)



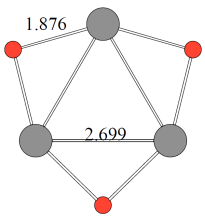
$Re_3O_3^-$ C_{2v} ($^5A_2$:3.65 eV)



$Re_3O_3^-$ C_s ($^7A''$:3.83 eV)



$Re_3O_3^-$ C_{2v} ($^1A_1$:4.29 eV)



$Re_3O_3^-$ D_{3h} ($^1A_1'$:5.36 eV)

Figure S2. Optimized structures (distances in angstroms and angles in degrees) and their relative energies for Re_3O_3 cluster.

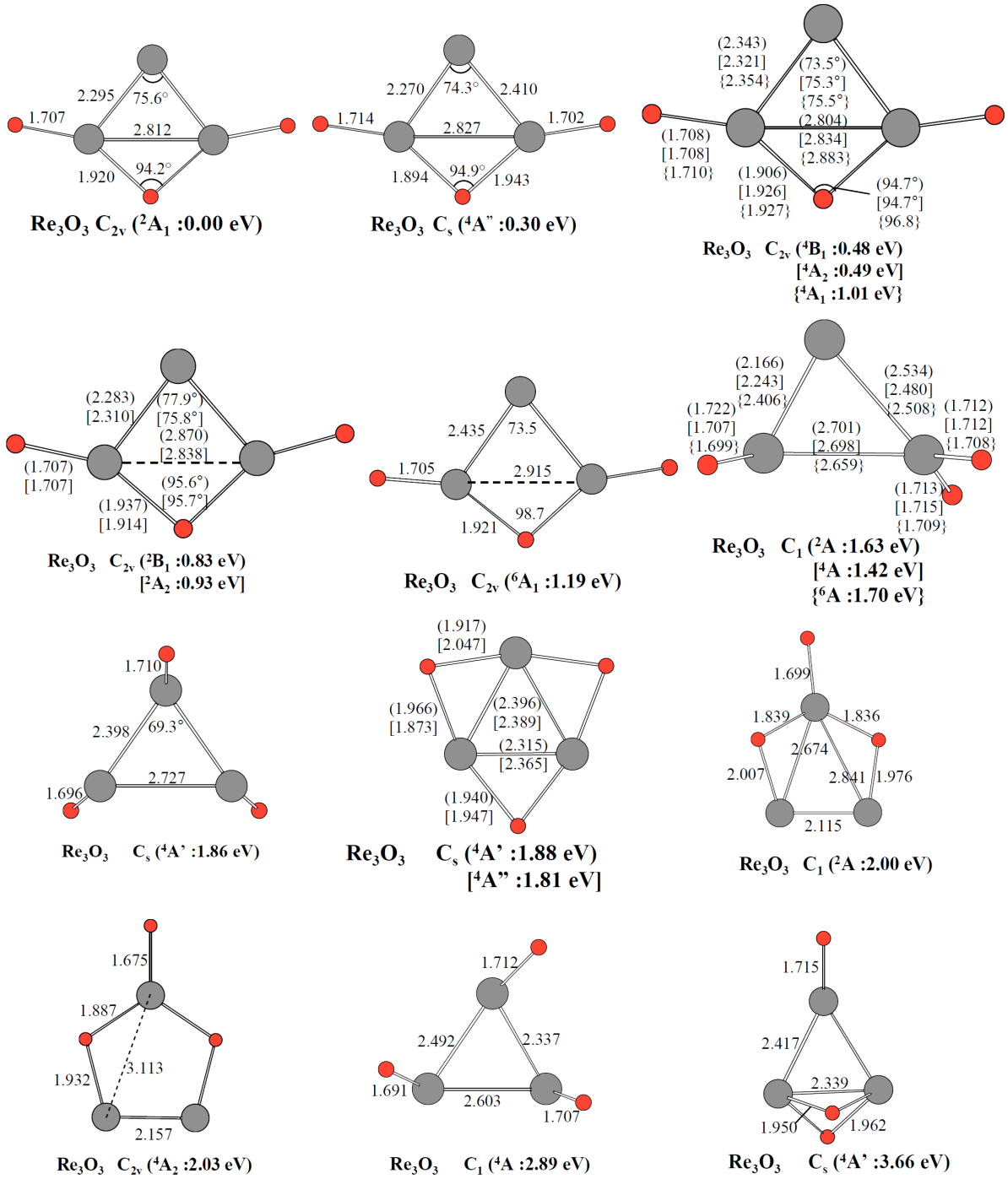
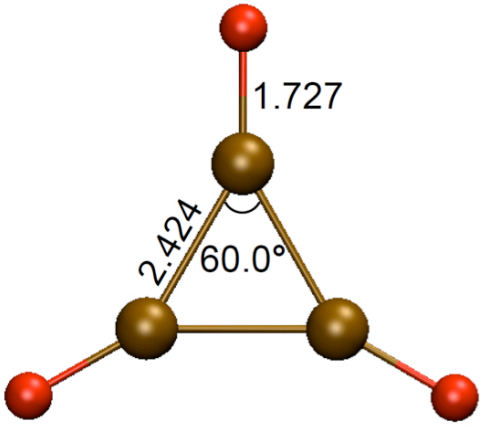


Figure S3. Molecular orbital pictures for the $Re_3O_3^-$ D_{3h} ($^3A_1'$) structure, which lies 3.06 eV above the global minimum at B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ level.



$Re_3O_3^-$ D_{3h} ($^3A_1'$: 3.06 eV)

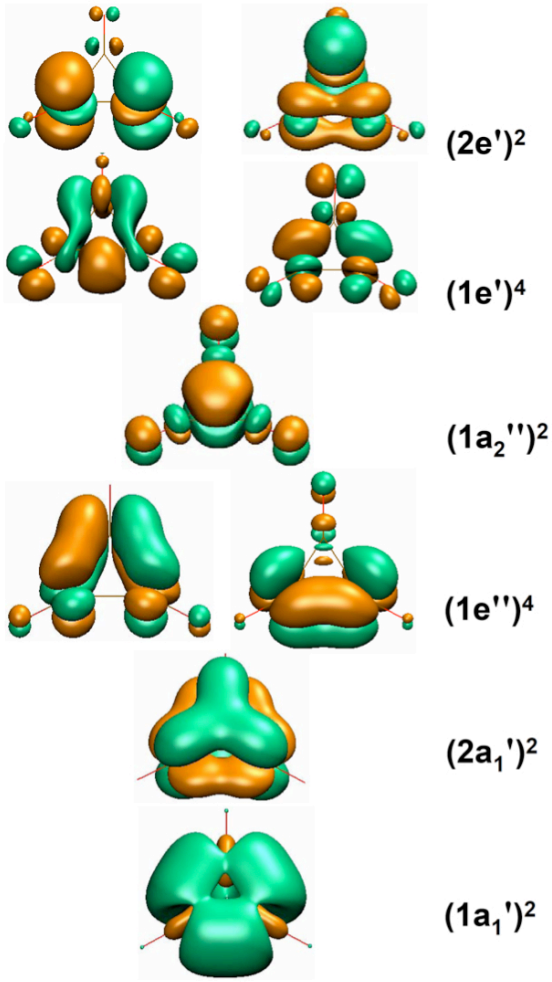
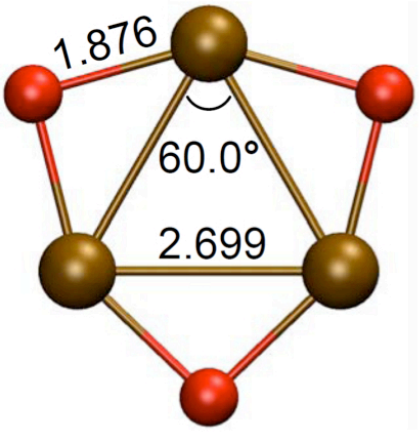


Figure S4. Molecular orbital pictures for the $Re_3O_3^-$ D_{3h} ($^1A_1'$) structure, which lies 5.36 eV above the global minimum at B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ level.



$Re_3O_3^-$ D_{3h} ($^1A_1'$: 5.36 eV)

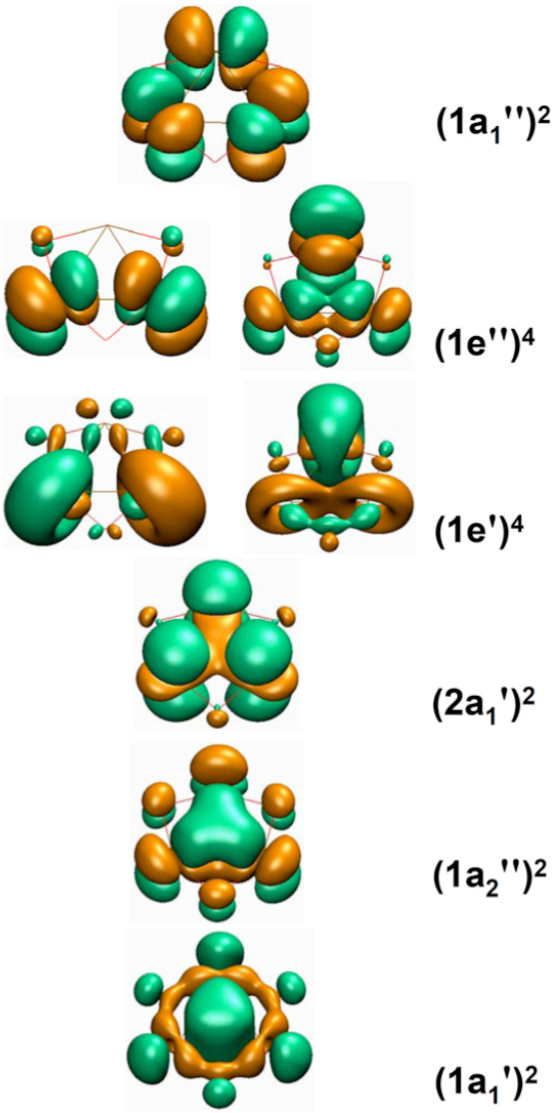


Table S1. Cartesian Coordinates for All Optimized Structures for $Re_3O_3^-$ and Re_3O_3 at B3LYP/Re/Stuttgart+2f1g/O/aug-cc-pVTZ Level.

(a) $Re_3O_3^-$

	x	y	z
$Re_3O_3^-$ (C_{2v} $^1A_1$ 0.00 eV)			
Re	0.000000	1.403968	-0.530269
Re	0.000000	0.000000	1.302774
Re	0.000000	-1.403968	-0.530269
O	0.000000	0.000000	-1.839219
O	0.000000	3.103265	-0.215868
O	0.000000	-3.103265	-0.215868
$Re_3O_3^-$ (C_s $^3A''$ 0.05 eV)			
Re	-1.421112	-0.481522	0.000000
Re	0.000000	1.303898	0.000000
Re	1.427331	-0.578406	0.000000
O	-0.066257	-1.824300	0.000000
O	-3.122358	-0.147669	0.000000
O	3.130307	-0.315257	0.000000
$Re_3O_3^-$ (C_s $^3A''$ 0.28 eV)			
Re	0.451255	-0.270984	1.417659
Re	-1.144063	0.666436	0.000000
Re	0.451255	-0.270984	-1.417659
O	1.362050	-1.173570	0.000000
O	0.451255	0.003340	3.126534
O	0.451255	0.003340	-3.126534
$Re_3O_3^-$ (C_{2v} $^5A_1$ 0.51 eV)			
Re	0.000000	1.426503	-0.544321
Re	0.000000	0.000000	1.352087
Re	0.000000	-1.426503	-0.544321
O	0.000000	0.000000	-1.826916
O	0.000000	3.142620	-0.321443
O	0.000000	-3.142620	-0.321443
$Re_3O_3^-$ (C_s $^3A'$ 0.85 eV)			
Re	-1.447446	-0.528157	0.000000
Re	0.000000	1.310229	0.000000
Re	1.447445	-0.528157	0.000000
O	0.000001	-1.800639	0.000000
O	-3.161163	-0.289897	0.000000
O	3.161165	-0.289914	0.000000
$Re_3O_3^-$ (C_1 ^1A 0.97 eV)			
Re	-0.470287	1.264645	0.134883
Re	1.452673	-0.283574	0.016967
Re	-1.212081	-0.706957	-0.261339
O	-2.351042	-1.415603	0.860504
O	1.847366	-1.411683	1.264570
O	2.657062	0.257466	-1.098615
$Re_3O_3^-$ (C_1 ^5A 1.07 eV)			
Re	-1.338828	-0.468467	0.018076
Re	1.376670	-0.602294	-0.173536
Re	0.133185	1.392349	0.052840
o	-2.218265	-0.727672	-1.456399
o	-1.959280	-0.976834	1.556340
o	2.574165	-1.310382	0.862119
$Re_3O_3^-$ (C_s $^3A''$ 1.25 eV)			
Re	-0.811076	1.060054	0.000000
Re	1.344133	0.587820	0.000000
Re	-0.653789	-1.357718	0.000000
o	-0.811076	-2.179861	1.515888
o	-0.811076	-2.179861	-1.515888
o	2.754023	1.639511	0.000000
$Re_3O_3^-$ (C_1 ^1A 1.34 eV)			
Re	-0.596135	1.136863	-0.175702
Re	-1.077716	-1.083283	0.065582
Re	1.426319	-0.184616	0.058328
O	0.586282	-1.861898	-0.347943
O	-1.198126	2.443608	0.808479
O	2.932461	0.646760	0.025015

$Re_3O_3^-$ (C_s $^5A'$ 1.41 eV)

Re	0.626165	-0.214533	1.341095
Re	-1.214662	0.551493	0.000000
Re	0.626165	-0.214533	-1.341095
o	0.626165	-1.692650	2.234621
o	0.626165	-1.692650	-2.234621
o	-1.605476	2.237534	0.000000

$Re_3O_3^-$ (C_1 ^3A 1.44 eV)

Re	-1.415711	-0.207770	-0.002278
Re	0.623095	1.210083	0.030519
Re	1.311376	-0.825871	0.001013
O	-1.995948	-0.647474	1.570394
O	-2.561382	0.564593	-1.041485
O	-0.306056	-1.571255	-0.803166

$Re_3O_3^-$ (C_1 ^3A 1.55 eV)

Re	-0.877177	-1.050805	0.268888
Re	-0.651127	1.240941	-0.194502
Re	1.429560	-0.224486	-0.162576
o	-1.530557	-2.019108	-0.999691
o	2.895011	-0.036256	0.742118
o	-0.438738	2.377397	1.084366

$Re_3O_3^-$ (C_s $^3A''$ 1.57 eV)

Re	1.167437	0.870382	0.000000
Re	-0.579372	-0.381874	1.220937
Re	-0.579372	-0.381874	-1.220937
O	1.077241	2.591912	0.000000
O	-0.579372	-1.795798	-2.220404
O	-0.579372	-1.795798	2.220404

$Re_3O_3^-$ (C_s $^5A'$ 1.66 eV)

Re	-0.659568	1.207394	0.000000
Re	0.409164	-0.815395	1.103831
Re	0.409164	-0.815395	-1.103831
o	0.409164	1.142068	-1.569627
o	0.409164	1.142068	1.569627
o	-2.306704	1.685206	0.000000

$Re_3O_3^-$ (C_{2v} $^5B_1$ 1.70 eV)

Re	0.000000	0.000000	1.732931
Re	0.000000	1.103673	-1.130879
Re	0.000000	-1.103673	-1.130879
o	0.000000	-1.614716	0.763657
o	0.000000	1.614716	0.763657
o	0.000000	0.000000	3.430433

$Re_3O_3^-$ (C_s $^7A'$ 1.79 eV)

Re	-0.232511	1.646780	0.000000
Re	0.153093	-1.079040	1.109981
Re	0.153093	-1.079040	-1.109981
o	0.153093	0.814659	-1.654747
o	0.153093	0.814659	1.654747
o	-0.996877	3.164114	0.000000

$Re_3O_3^-$ (C_s $^7A''$ 1.96 eV)

Re	-0.680542	1.159643	0.000000
Re	0.420134	-0.789182	1.175867
Re	0.420134	-0.789182	-1.175867
o	0.420134	1.155136	-1.569584
o	0.420134	1.155136	1.569584
o	-2.337689	1.615249	0.000000

$Re_3O_3^-$ (C_1 ^3A 2.05eV)

Re	1.433994	0.000000	0.022366
Re	-0.831774	1.127915	-0.035621
Re	-0.831774	-1.127915	-0.035621
O	2.264141	-0.000001	-1.494456
O	2.254404	0.000001	1.546973
O	-2.366468	0.000000	0.405691

$Re_3O_3^-$ (C_{3v} $^3A_1$ 2.08 eV)

Re	0.000000	1.373175	-0.033261
Re	-1.189205	-0.686588	-0.033261
Re	1.189205	-0.686588	-0.033261
o	1.901356	1.097749	0.311819
o	0.000000	-2.195497	0.311819
o	-1.901356	1.097749	0.311819

$Re_3O_3^-$ (C_s $^5A'$ 2.19 eV)

Re	-0.053829	-0.691450	1.196394
Re	0.157218	1.403012	0.000000
Re	-0.053829	-0.691450	-1.196394
o	-0.356982	-2.212616	0.000000
o	-0.053829	1.012033	-2.014944
o	-0.053829	1.012033	2.014944

$Re_3O_3^-$ (C_s $^1A'$ 2.27 eV)

Re	-0.085768	1.276017	0.000000
Re	-0.001144	-0.649271	1.244528
Re	-0.001144	-0.649271	-1.244528
o	-0.001144	1.056587	-2.035880
o	0.827810	-1.902002	0.000000
o	-0.001144	1.056587	2.035880

$Re_3O_3^-$ (C_{2v} $^3B_2$ 2.31 eV)

Re	0.000000	0.000000	1.817455
Re	0.000000	1.052293	-1.176329
Re	0.000000	-1.052293	-1.176329
o	0.000000	-1.507770	0.750071
o	0.000000	1.507770	0.750071
o	0.000000	0.000000	3.517379

$Re_3O_3^-$ (C_s $^5A''$ 2.35 eV)

Re	1.300609	0.042268	0.000000
Re	-0.683760	-0.200754	1.304654
Re	-0.683760	-0.200754	-1.304654
O	1.994805	1.636828	0.000000
O	-0.683760	0.865524	-2.661830
O	-0.683760	0.865524	2.661830

$Re_3O_3^-$ (C_{2v} $^5A_1$ 2.35 eV)

Re	0.000000	0.000000	1.393391
Re	0.000000	1.195497	-0.681868
Re	0.000000	-1.195497	-0.681868
o	0.000000	-2.061057	0.984800
o	0.000000	0.000000	-2.247625
o	0.000000	2.061057	0.984800

$Re_3O_3^-$ (C_s $^1A'$ 2.45 eV)

Re	-0.748127	1.194124	0.000000
Re	0.450824	-0.807148	1.114338
Re	0.450824	-0.807148	-1.114338
o	0.450824	1.061950	-1.505050
o	0.450824	1.061950	1.505050
o	-2.340905	1.815208	0.000000

$Re_3O_3^-$ (C_s $^1A'$ 2.49 eV)

Re	-0.428256	1.321165	0.000000
Re	0.297036	-0.960655	1.051710
Re	0.297036	-0.960655	-1.051710
O	0.297036	2.071552	1.410430
O	0.297036	2.071552	-1.410430
O	-2.148590	1.483261	0.000000

$Re_3O_3^-$ (D_{3h} $^3A_1$' 3.06 eV)

Re	0.000000	1.399206	0.000000
Re	1.211748	-0.699603	0.000000
Re	-1.211748	-0.699603	0.000000
o	0.000000	3.126660	0.000000
o	-2.707767	-1.563330	0.000000
o	2.707767	-1.563330	0.000000

$Re_3O_3^-$ (C_{2v} $^1A_1$ 3.28 eV)

Re	0.000000	0.000000	1.383503
Re	0.000000	1.132912	-0.689097
Re	0.000000	-1.132912	-0.689097
o	0.000000	-1.950984	1.132741
o	0.000000	0.000000	-2.315255
o	0.000000	1.950984	1.132741

$Re_3O_3^-$ (C_{2v} $^5A_2$ 3.65 eV)

Re	0.000000	1.268869	-0.688691
Re	0.000000	0.000000	1.371110
Re	0.000000	-1.268869	-0.688691
o	-1.240393	0.000000	-1.531606
o	1.240393	0.000000	-1.531606
o	0.000000	0.000000	3.122020

$Re_3O_3^-$ (C_s $^7A''$ 3.83 eV)

Re	-0.155951	-0.663624	1.285141
Re	0.406010	1.318069	0.000000
Re	-0.155951	-0.663624	-1.285141
o	0.840471	-1.755068	0.000000
o	-1.566776	-1.120664	0.000000
o	-0.155951	2.961787	0.000000

$Re_3O_3^-$ (C_{2v} $^1A_1$ 4.29 eV)

Re	0.000000	1.199939	-0.677833
Re	0.000000	0.000000	1.345203
Re	0.000000	-1.199939	-0.677833
o	-1.331727	0.000000	-1.503500
o	1.331727	0.000000	-1.503500
o	0.000000	0.000000	3.105083

$Re_3O_3^-$ (D_{3h} $^1A_1$' 5.36 eV)

Re	0.000000	1.558476	0.000000
Re	1.349679	-0.779238	0.000000
Re	-1.349679	-0.779238	0.000000
o	-1.802856	1.040879	0.000000
o	0.000000	-2.081759	0.000000
o	1.802856	1.040879	0.000000

(b) Re_3O_3

Re_3O_3 (C_{2v} $^2A_1$ 0.00 eV)

	x	y	z
Re	0.000000	1.406000	-0.525145
Re	0.000000	0.000000	1.288476
Re	0.000000	-1.406000	-0.525145
O	0.000000	0.000000	-1.832466
O	0.000000	3.081623	-0.200262
O	0.000000	-3.081623	-0.200262

Re_3O_3 (C_s ^4A" 0.30 eV)

Re	-1.406889	-0.453066	0.000000
Re	0.000000	1.327910	0.000000
Re	1.415142	-0.623222	0.000000
O	-0.106570	-1.830974	0.000000
O	-3.079309	-0.078438	0.000000
O	3.108510	-0.449547	0.000000

Re_3O_3 (C_{2v} $^4B_1$ 0.48 eV)

Re	0.000000	1.401998	-0.539216
Re	0.000000	0.000000	1.338106
Re	0.000000	-1.401998	-0.539216
O	0.000000	0.000000	-1.830578
O	0.000000	3.093576	-0.301932
O	0.000000	-3.093576	-0.301932

Re_3O_3 (C_{2v} $^4A_2$ 0.49 eV)

Re	0.000000	1.417064	-0.534708
Re	0.000000	0.000000	1.302951
Re	0.000000	-1.417064	-0.534708
O	0.000000	0.000000	-1.838965
O	0.000000	3.086394	-0.175211
O	0.000000	-3.086394	-0.175211

Re_3O_3 (C_{2v} $^4A_1$ 1.01 eV)

Re	0.000000	1.441400	-0.533688
Re	0.000000	0.000000	1.327260
Re	0.000000	-1.441400	-0.533688
O	0.000000	0.000000	-1.813079
O	0.000000	3.136665	-0.311667
O	0.000000	-3.136665	-0.311667

Re_3O_3 (C_{2v} $^2B_1$ 0.83 eV)

Re	0.000000	1.434753	-0.519306
Re	0.000000	0.000000	1.256809
Re	0.000000	-1.434753	-0.519306
O	0.000000	0.000000	-1.819969
O	0.000000	3.093323	-0.112813
O	0.000000	-3.093323	-0.112813

Re_3O_3 (C_{2v} $^2A_2$ 0.93 eV)

Re	0.000000	1.419047	-0.523395
Re	0.000000	0.000000	1.299482
Re	0.000000	-1.419047	-0.523395
O	0.000000	0.000000	-1.807975
O	0.000000	3.108654	-0.280505
O	0.000000	-3.108654	-0.280505

Re_3O_3 (C_{2v} $^6A_1$ 1.19 eV)

Re	0.000000	1.457350	-0.560025

Re	0.000000	0.000000	1.390707
Re	0.000000	-1.457350	-0.560025
O	0.000000	0.000000	-1.811565
O	0.000000	3.151060	-0.362924
O	0.000000	-3.151060	-0.362924

Re_3O_3 (C_1 ^{2}A 1.63 eV)

Re	-0.560699	1.275027	0.008553
Re	1.476960	-0.230299	0.029988
Re	-1.155747	-0.800416	-0.164550
O	-2.263035	-1.415897	1.001300
O	2.156788	-0.362801	1.595548
O	2.351425	-0.511719	-1.415513

Re_3O_3 (C_1 ^{4}A 1.42 eV)

Re	-0.472312	1.314751	0.053682
Re	1.425890	-0.280779	0.020997
Re	-1.213929	-0.785785	-0.211926
O	-2.006718	-1.364421	1.184984
O	2.122041	-0.649579	1.540749
O	2.325466	-0.312748	-1.439040

Re_3O_3 (C_1 ^{6}A 1.70 eV)

Re	-0.351194	1.455962	0.075068
Re	1.362655	-0.374433	0.006156
Re	-1.260536	-0.754656	-0.198295
O	-1.922870	-1.758043	1.002543
O	1.977161	-0.849625	1.527410
O	2.280789	-0.456771	-1.432410

Re_3O_3 (C_s ^{4}A' 1.86 eV)

Re	0.627875	-0.170080	1.363721
Re	-1.233774	0.482957	0.000000
Re	0.627875	-0.170080	-1.363721
O	0.627875	-1.758122	1.957737
O	0.627875	-1.758122	-1.957737
O	-1.461772	2.177513	0.000000

Re_3O_3 (C_s ^{4}A' 1.88 eV)

Re	-0.345518	1.356314	0.000000
Re	0.117973	-0.689303	1.157623
Re	0.117973	-0.689303	-1.157623
O	0.117973	1.151095	-1.848650
O	0.791292	-2.093209	0.000000
O	0.117973	1.151095	1.848650

Re_3O_3 (C_s ^{4}A" 1.81 eV)

Re	-0.248178	1.369447	0.000000
Re	0.078959	-0.680357	1.182501
Re	0.078959	-0.680357	-1.182501
O	0.078959	1.010310	-1.988715
O	0.688276	-2.102487	0.000000
O	0.078959	1.010310	1.988715

Re_3O_3 (C_1 ^{2}A 2.00 eV)

Re	1.527182	-0.109708	0.011984
Re	-0.848245	1.111968	-0.117091
Re	-1.179918	-0.966418	0.097130
O	0.573007	-1.553231	-0.601933
O	0.906410	1.429311	0.805145
O	3.217282	-0.212090	-0.128427

Re_3O_3 (C_{2v} $^4A_2$ 2.03 eV)

Re	0.000000	0.000000	1.773045
Re	0.000000	1.078546	-1.147404
Re	0.000000	-1.078546	-1.147404
O	0.000000	-1.567134	0.721686
O	0.000000	1.567134	0.721686
O	0.000000	0.000000	3.448156

Re_3O_3 (C_1 ^{4}A 2.89 eV)

Re	0.429365	1.249965	-0.163039
Re	1.032562	-1.007948	-0.135590
Re	-1.484182	-0.343810	-0.083071
O	1.379314	2.008947	1.041667
O	-2.527334	0.360019	1.046695
O	1.356661	-1.414650	1.490074

Re_3O_3 (C_s ^{4}A' 3.66 eV)

Re	0.160198	-0.681889	1.169324
Re	-0.435097	1.347930	0.000000
Re	0.160198	-0.681889	-1.169324
O	1.709370	-0.872661	0.000000
O	-0.794239	-1.935426	0.000000
O	0.160198	2.956667	0.000000