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Supporting information for article:

Do the basic crystal chemistry principles agree with a plethora of recent quantum chemistry data?

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Supporting Information

Do the Basic Crystal Chemistry Principles Agree with a Plethora of Recent Quantum Chemistry Data?

Elena Levi*, Doron Aurbach and Carlo Gatti*

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Figure S1. Direct correlation between bond order and the average bond energy for three important atom pairs (The data from ref.[1]).

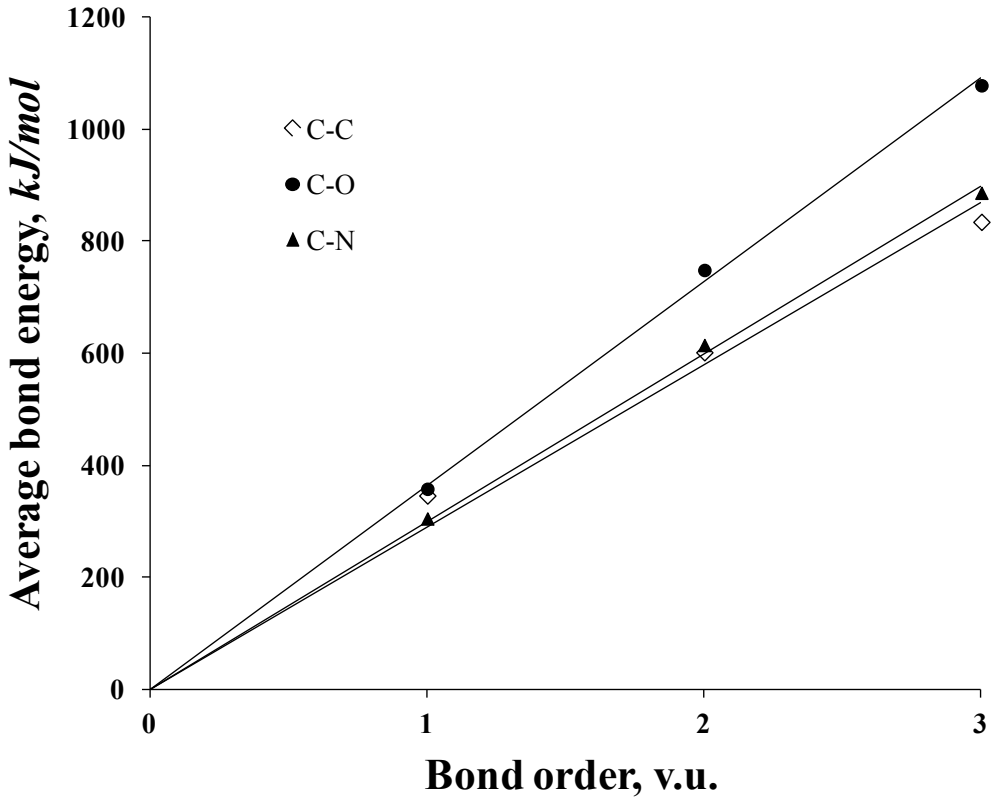
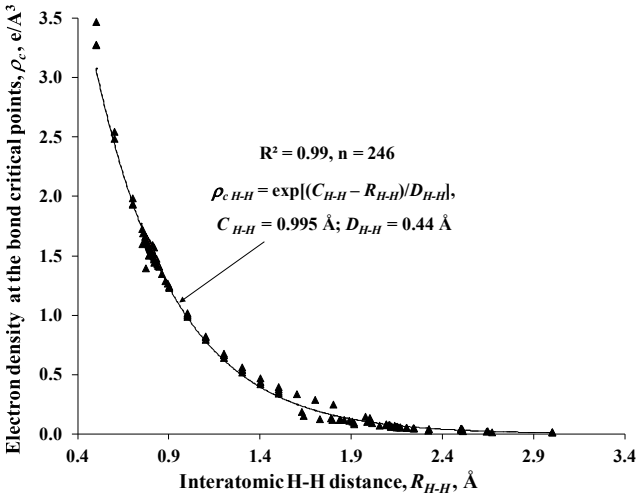
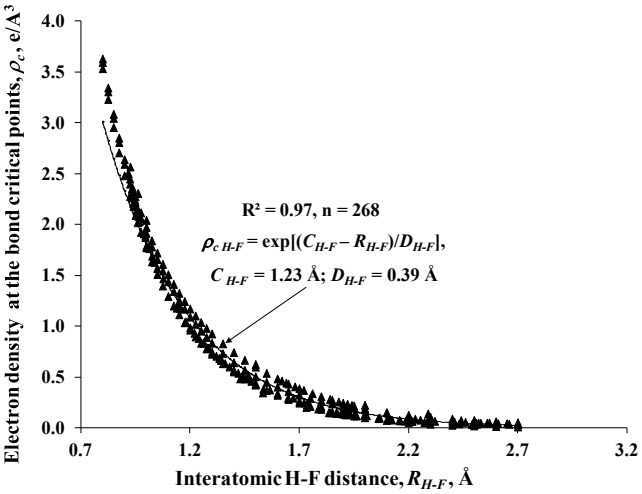
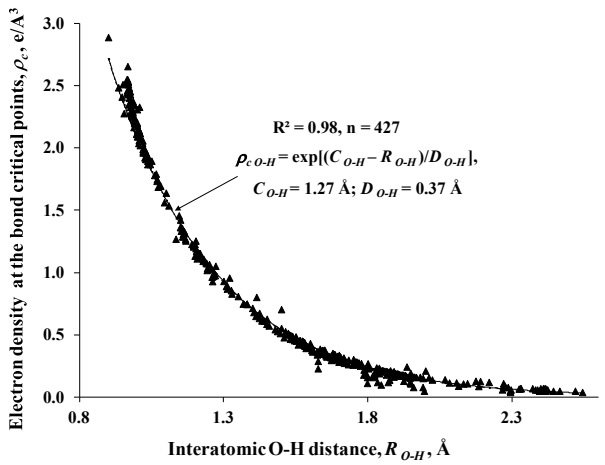
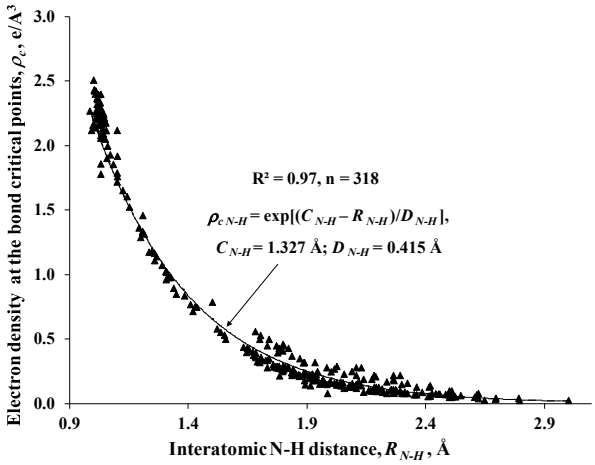


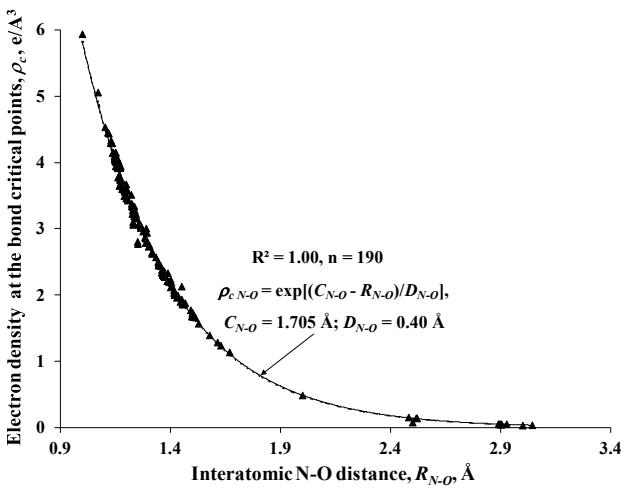
Figure S2. Exponential correlations between electron density, $\rho_{c\ ij}$, and the interatomic distances. The points are quantum chemistry data available in literature.

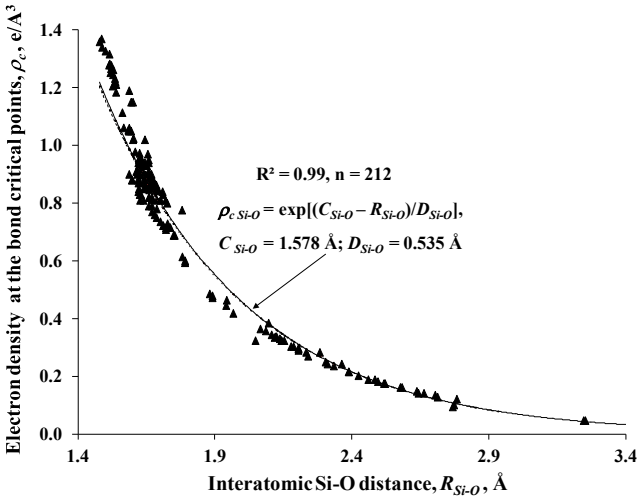


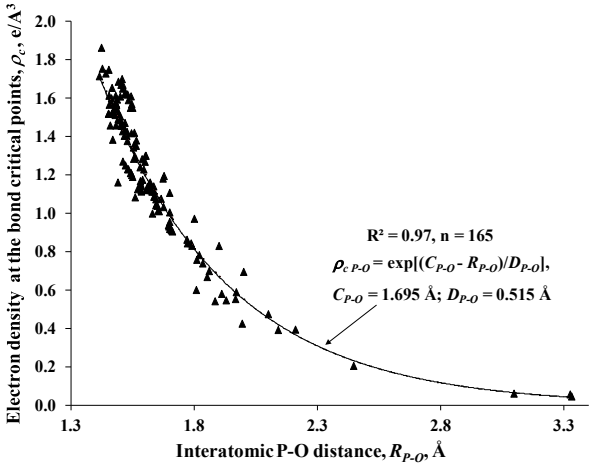


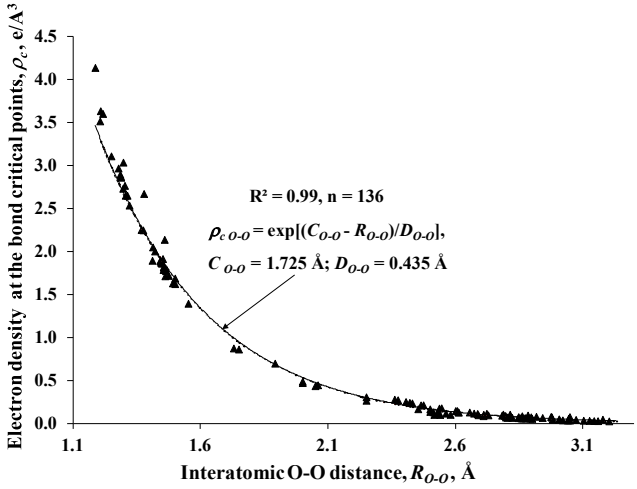


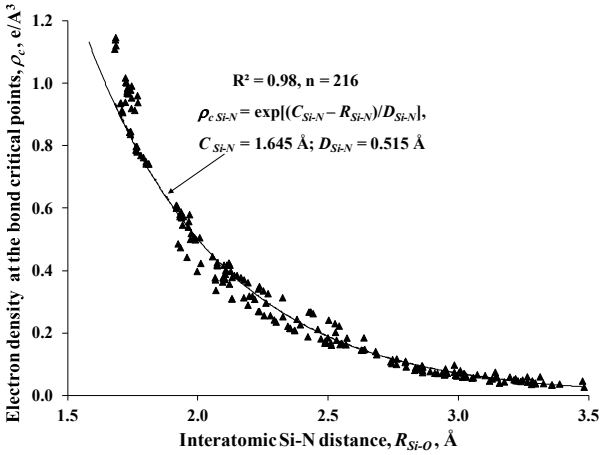


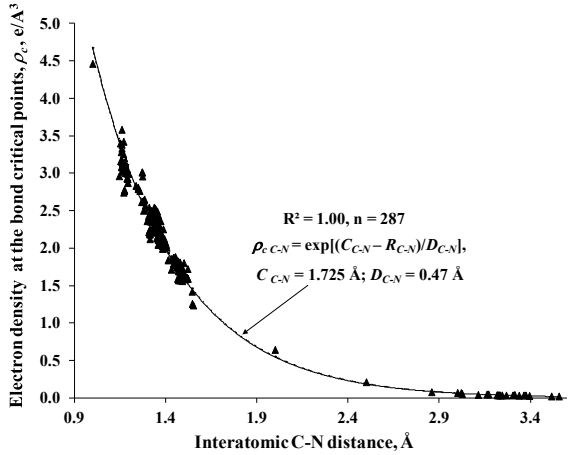


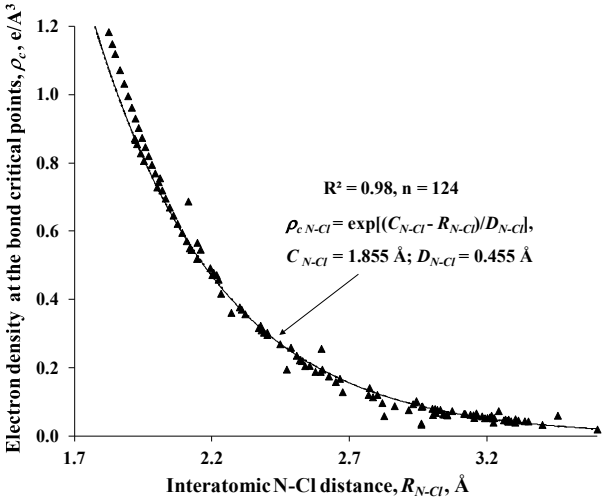


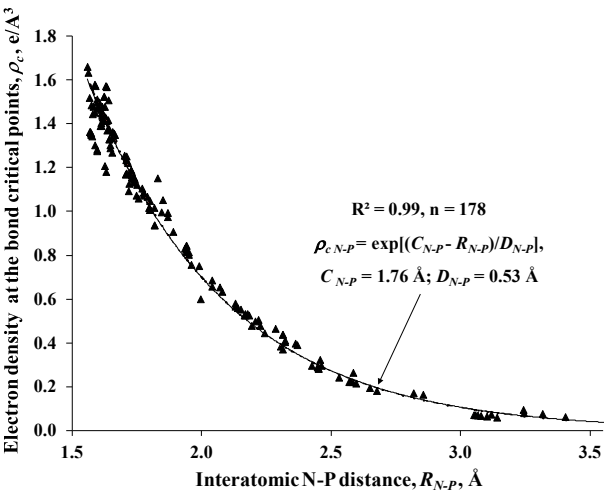

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic P-O distance, R_{P-O}, Å
R² = 0.97, n = 165
$\rho_{c\,P-O} = \exp[(C_{P-O} - R_{P-O})/D_{P-O}]$,
C_{P-O} = 1.695 Å; D_{P-O} = 0.515 Å

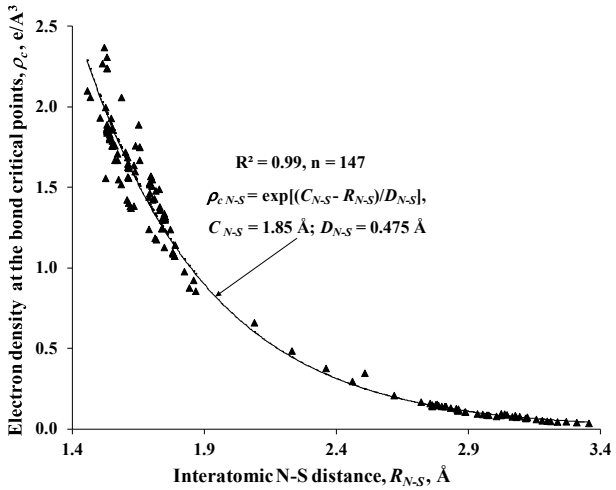

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic O-O distance, R_{O-O}, Å
R² = 0.99, n = 136
$\rho_{c\,O-O} = \exp[(C_{O-O} - R_{O-O})/D_{O-O}]$,
C_{O-O} = 1.725 Å; D_{O-O} = 0.435 Å

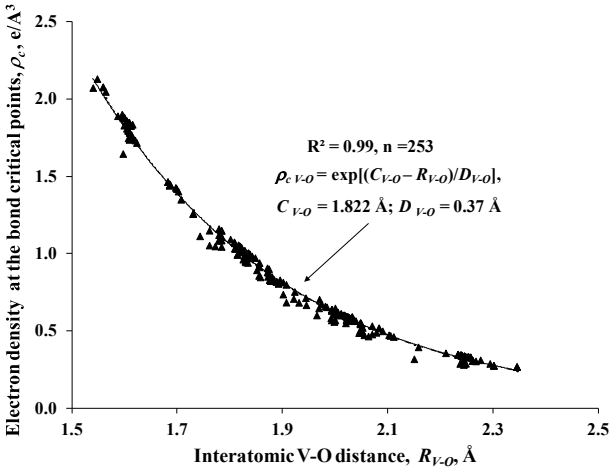

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic Si-N distance, R_{Si-O}, Å
R² = 0.98, n = 216
$\rho_{c\,Si-N} = \exp[(C_{Si-N} - R_{Si-N})/D_{Si-N}]$,
C_{Si-N} = 1.645 Å; D_{Si-N} = 0.515 Å

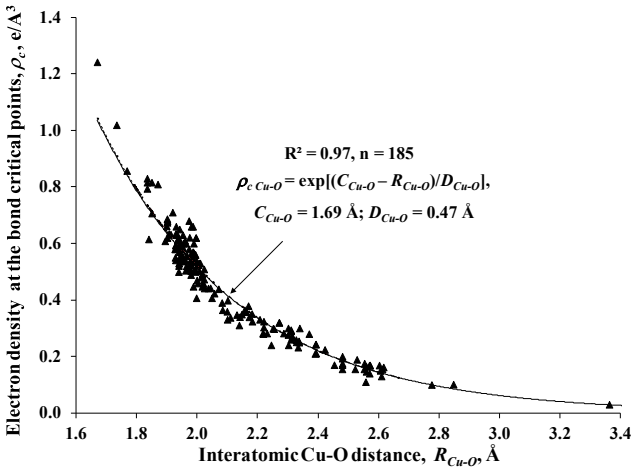

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic C-N distance, Å
R² = 1.00, n = 287
$\rho_{c\,C-N} = \exp[(C_{C-N} - R_{C-N})/D_{C-N}]$,
C_{C-N} = 1.725 Å; D_{C-N} = 0.47 Å

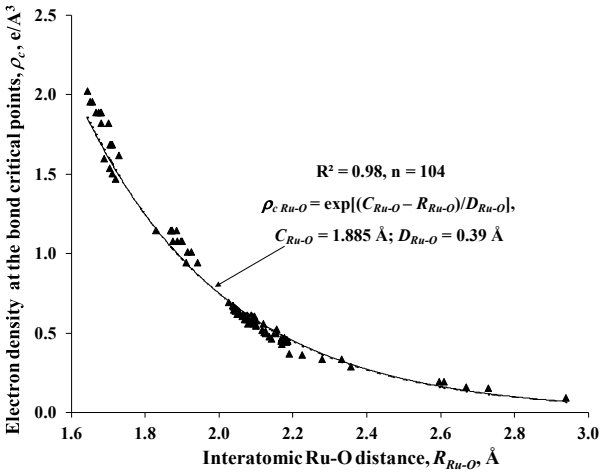

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic N-Cl distance, R_{N-Cl}, Å
R² = 0.98, n = 124
$\rho_{c\,N-Cl} = \exp[(C_{N-Cl} - R_{N-Cl})/D_{N-Cl}]$,
C_{N-Cl} = 1.855 Å; D_{N-Cl} = 0.455 Å

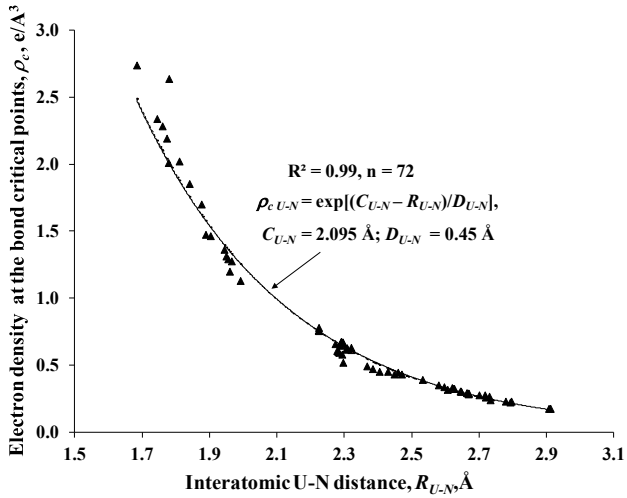

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic N-P distance, R_{N-P}, Å
R² = 0.99, n = 178
$\rho_{c\,N-P} = \exp[(C_{N-P} - R_{N-P})/D_{N-P}]$,
C_{N-P} = 1.76 Å; D_{N-P} = 0.53 Å

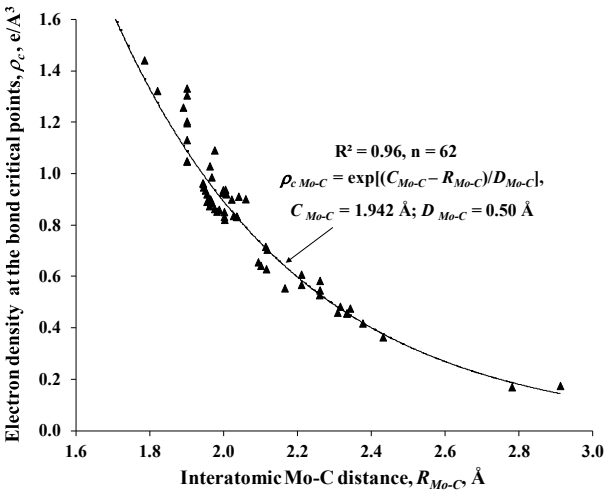

Electron density at the bond critical points, ρ_c, e/A^3
R² = 0.99, n = 147
$\rho_{c\ N\text{-}S} = \exp[(C_{N\text{-}S} - R_{N\text{-}S})/D_{N\text{-}S}]$,
$C_{N\text{-}S}$ = 1.85 Å; $D_{N\text{-}S}$ = 0.475 Å
Interatomic N-S distance, $R_{N\text{-}S}$, Å

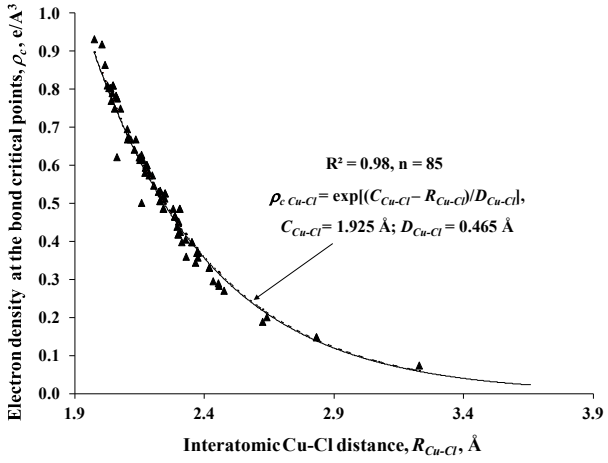

Electron density at the bond critical points, ρ_c, e/A^3
R² = 0.99, n =253
$\rho_{c\ V\text{-}O} = \exp[(C_{V\text{-}O} - R_{V\text{-}O})/D_{V\text{-}O}]$,
$C_{V\text{-}O}$ = 1.822 Å; $D_{V\text{-}O}$ = 0.37 Å
Interatomic V-O distance, $R_{V\text{-}O}$, Å

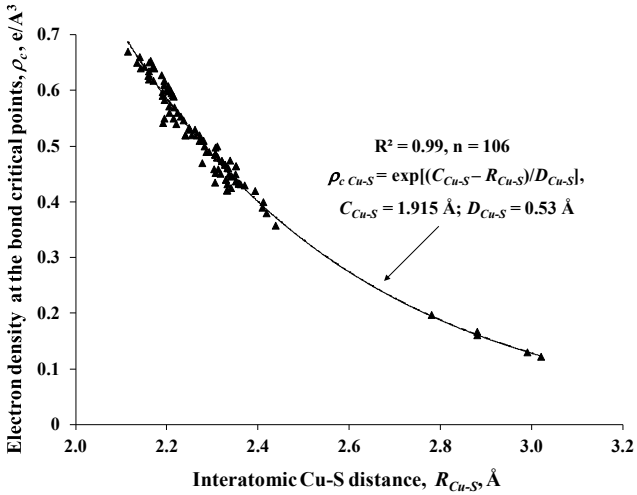

Electron density at the bond critical points, ρ_c, e/A^3
R² = 0.97, n = 185
$\rho_{c\ Cu\text{-}O} = \exp[(C_{Cu\text{-}O} - R_{Cu\text{-}O})/D_{Cu\text{-}O}]$,
$C_{Cu\text{-}O}$ = 1.69 Å; $D_{Cu\text{-}O}$ = 0.47 Å
Interatomic Cu-O distance, $R_{Cu\text{-}O}$, Å

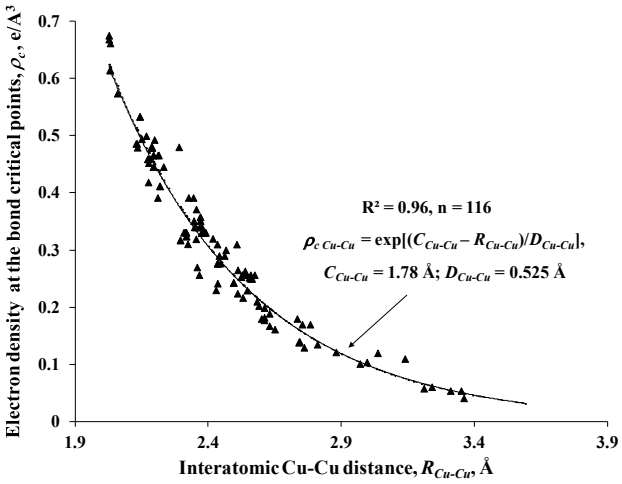

Electron density at the bond critical points, ρ_c, e/A^3
R² = 0.98, n = 104
$\rho_{c\ Ru\text{-}O} = \exp[(C_{Ru\text{-}O} - R_{Ru\text{-}O})/D_{Ru\text{-}O}]$,
$C_{Ru\text{-}O}$ = 1.885 Å; $D_{Ru\text{-}O}$ = 0.39 Å
Interatomic Ru-O distance, $R_{Ru\text{-}O}$, Å

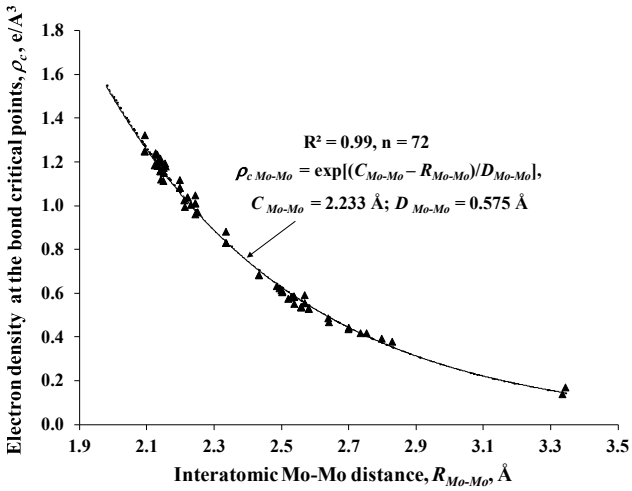

Electron density at the bond critical points, ρ_c, e/A^3
R² = 0.99, n = 72
$\rho_{c\ U\text{-}N} = \exp[(C_{U\text{-}N} - R_{U\text{-}N})/D_{U\text{-}N}]$,
$C_{U\text{-}N}$ = 2.095 Å; $D_{U\text{-}N}$ = 0.45 Å
Interatomic U-N distance, $R_{U\text{-}N}$, Å


Electron density at the bond critical points, ρ_c, e/A^3
R² = 0.96, n = 62
$\rho_{c\ Mo\text{-}C} = \exp[(C_{Mo\text{-}C} - R_{Mo\text{-}C})/D_{Mo\text{-}C}]$,
$C_{Mo\text{-}C}$ = 1.942 Å; $D_{Mo\text{-}C}$ = 0.50 Å
Interatomic Mo-C distance, $R_{Mo\text{-}C}$, Å


Electron density at the bond critical points, ρ_c, e/A^3
Interatomic Cu-Cl distance, R_{Cu-Cl}, Å
R² = 0.98, n = 85
$\rho_{c\ Cu-Cl} = \exp[(C_{Cu-Cl} - R_{Cu-Cl})/D_{Cu-Cl}]$,
C_{Cu-Cl} = 1.925 Å; D_{Cu-Cl} = 0.465 Å


Electron density at the bond critical points, ρ_c, e/A^3
Interatomic Cu-S distance, R_{Cu-S}, Å
R² = 0.99, n = 106
$\rho_{c\ Cu-S} = \exp[(C_{Cu-S} - R_{Cu-S})/D_{Cu-S}]$,
C_{Cu-S} = 1.915 Å; D_{Cu-S} = 0.53 Å


Electron density at the bond critical points, ρ_c, e/A^3
Interatomic Cu-Cu distance, R_{Cu-Cu}, Å
R² = 0.96, n = 116
$\rho_{c\ Cu-Cu} = \exp[(C_{Cu-Cu} - R_{Cu-Cu})/D_{Cu-Cu}]$,
C_{Cu-Cu} = 1.78 Å; D_{Cu-Cu} = 0.525 Å


Electron density at the bond critical points, ρ_c, e/A^3
Interatomic Mo-Mo distance, R_{Mo-Mo}, Å
R² = 0.99, n = 72
$\rho_{c\ Mo-Mo} = \exp[(C_{Mo-Mo} - R_{Mo-Mo})/D_{Mo-Mo}]$,
C_{Mo-Mo} = 2.233 Å; D_{Mo-Mo} = 0.575 Å

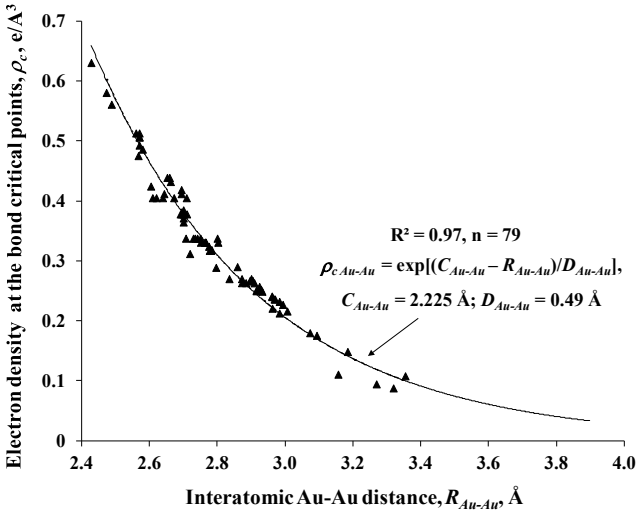
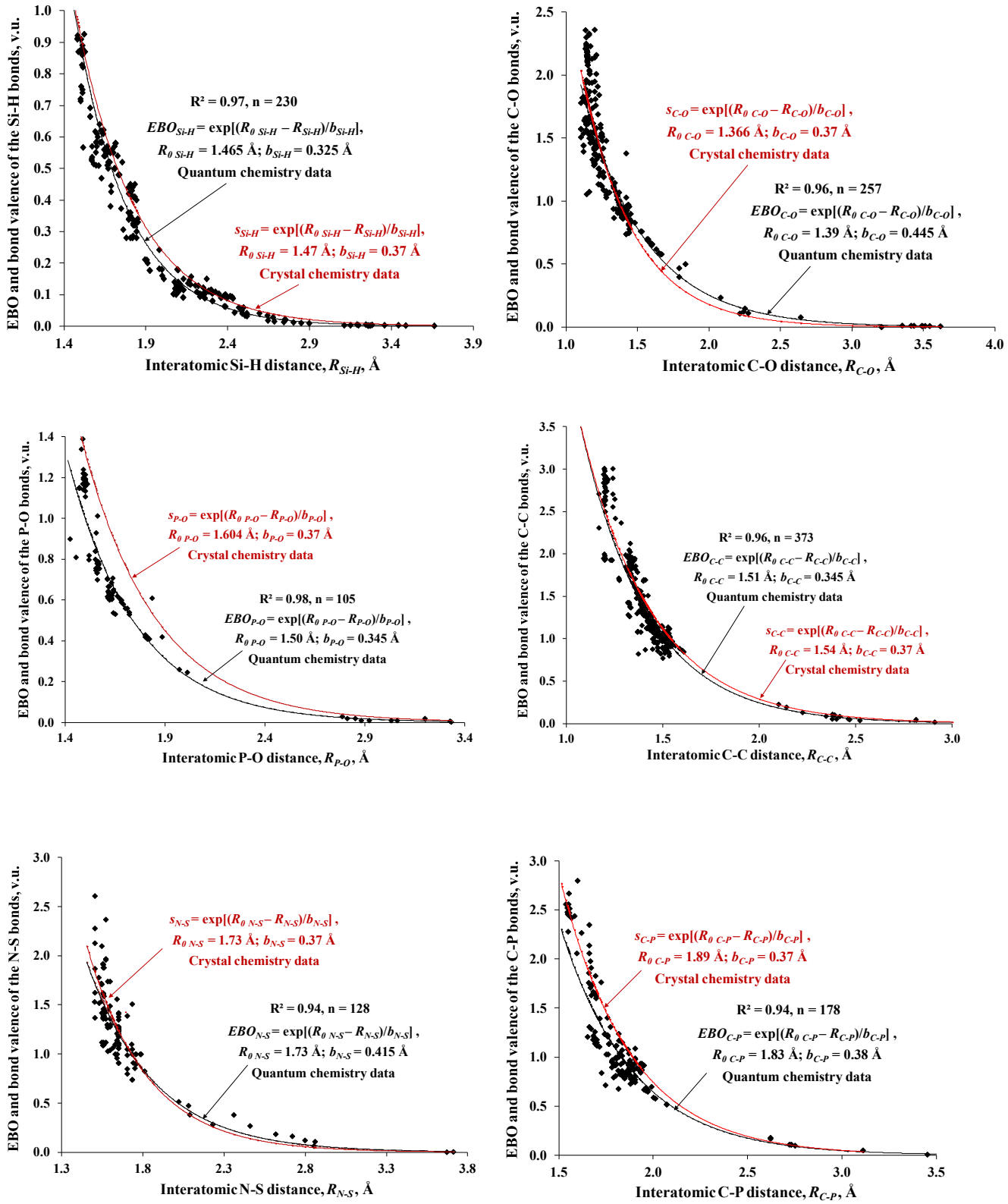
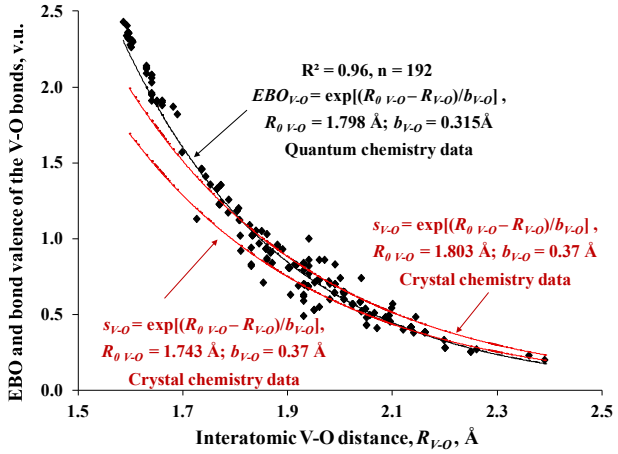
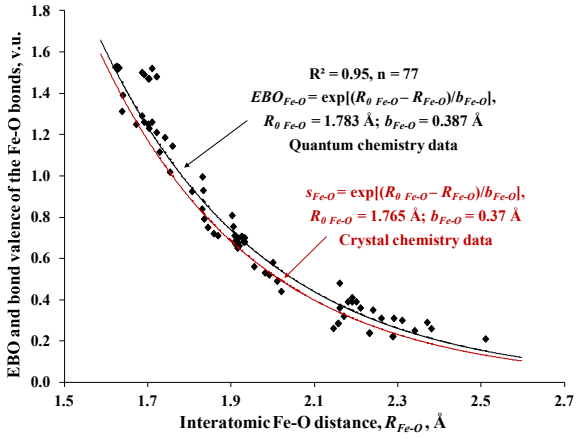
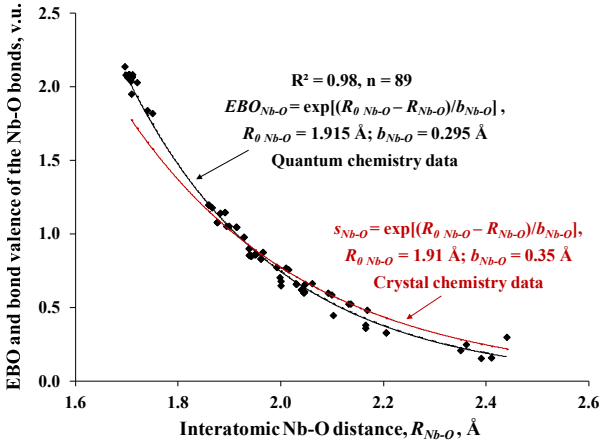

Electron density at the bond critical points, ρ_c, e/A^3
Interatomic Au-Au distance, R_{Au-Au}, Å
R² = 0.97, n = 79
$\rho_{c\ Au-Au} = \exp[(C_{Au-Au} - R_{Au-Au})/D_{Au-Au}]$,
C_{Au-Au} = 2.225 Å; D_{Au-Au} = 0.49 Å

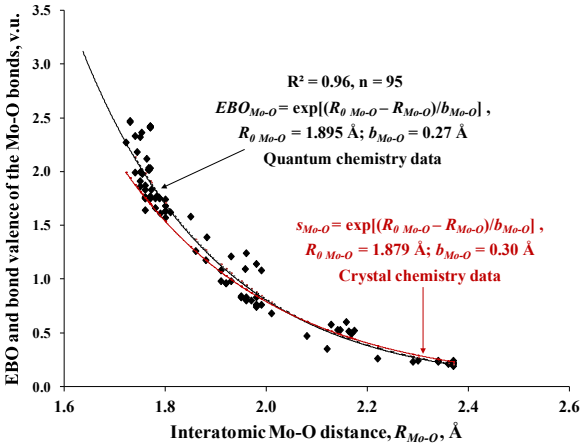
Figure S3. Exponential correlations between effective bond order, BO_{ij}, and the interatomic distances. The points are the quantum chemistry data available in literature. The crystal chemistry curves marked in red are presented for comparison.

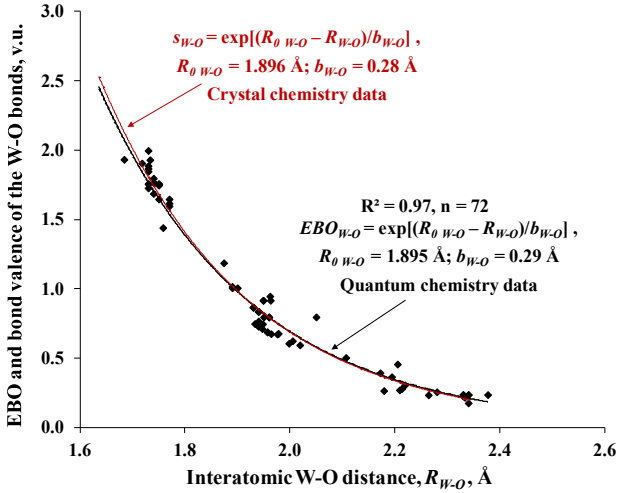


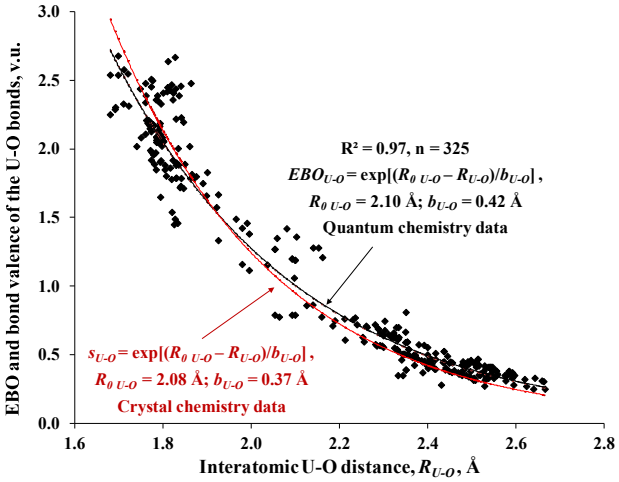

EBO and bond valence of the V-O bonds, v.u.
Interatomic V-O distance, R_{V-O}, Å
R² = 0.96, n = 192
$EBO_{V-O} = \exp[(R_{0\ V-O} - R_{V-O})/b_{V-O}]$,
$R_{0\ V-O}$ = 1.798 Å; b_{V-O} = 0.315Å
Quantum chemistry data
$s_{V-O} = \exp[(R_{0\ V-O} - R_{V-O})/b_{V-O}]$,
$R_{0\ V-O}$ = 1.803 Å; b_{V-O} = 0.37 Å
Crystal chemistry data
$s_{V-O} = \exp[(R_{0\ V-O} - R_{V-O})/b_{V-O}]$,
$R_{0\ V-O}$ = 1.743 Å; b_{V-O} = 0.37 Å
Crystal chemistry data

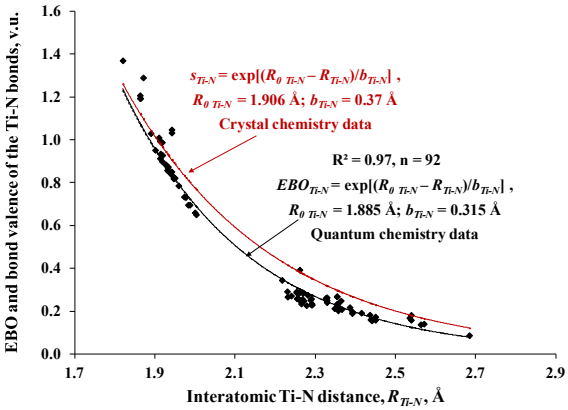

EBO and bond valence of the Fe-O bonds, v.u.
Interatomic Fe-O distance, R_{Fe-O}, Å
R² = 0.95, n = 77
$EBO_{Fe-O} = \exp[(R_{0\ Fe-O} - R_{Fe-O})/b_{Fe-O}]$,
$R_{0\ Fe-O}$ = 1.783 Å; b_{Fe-O} = 0.387 Å
Quantum chemistry data
$s_{Fe-O} = \exp[(R_{0\ Fe-O} - R_{Fe-O})/b_{Fe-O}]$,
$R_{0\ Fe-O}$ = 1.765 Å; b_{Fe-O} = 0.37 Å
Crystal chemistry data

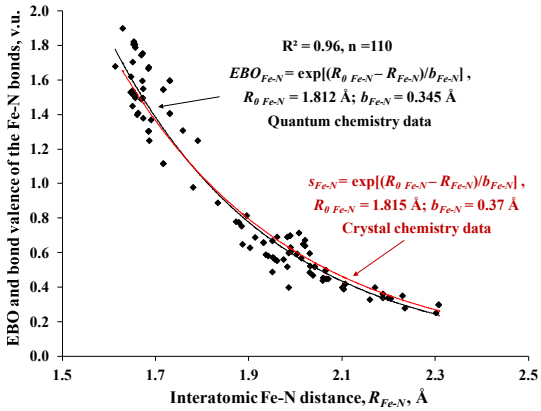

EBO and bond valence of the Nb-O bonds, v.u.
Interatomic Nb-O distance, R_{Nb-O}, Å
R² = 0.98, n = 89
$EBO_{Nb-O} = \exp[(R_{0\ Nb-O} - R_{Nb-O})/b_{Nb-O}]$,
$R_{0\ Nb-O}$ = 1.915 Å; b_{Nb-O} = 0.295 Å
Quantum chemistry data
$s_{Nb-O} = \exp[(R_{0\ Nb-O} - R_{Nb-O})/b_{Nb-O}]$,
$R_{0\ Nb-O}$ = 1.91 Å; b_{Nb-O} = 0.35 Å
Crystal chemistry data

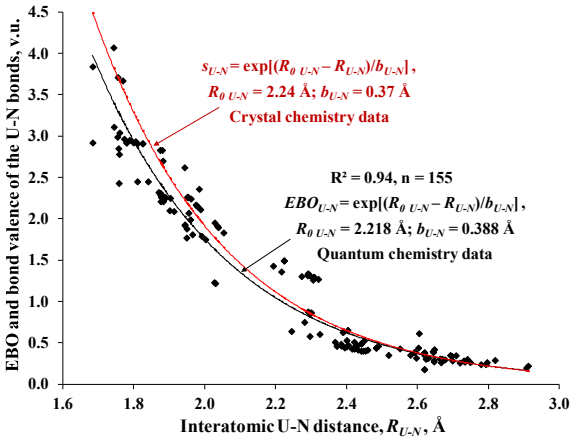

EBO and bond valence of the Mo-O bonds, v.u.
Interatomic Mo-O distance, R_{Mo-O}, Å
R² = 0.96, n = 95
$EBO_{Mo-O} = \exp[(R_{0\ Mo-O} - R_{Mo-O})/b_{Mo-O}]$,
$R_{0\ Mo-O}$ = 1.895 Å; b_{Mo-O} = 0.27 Å
Quantum chemistry data
$s_{Mo-O} = \exp[(R_{0\ Mo-O} - R_{Mo-O})/b_{Mo-O}]$,
$R_{0\ Mo-O}$ = 1.879 Å; b_{Mo-O} = 0.30 Å
Crystal chemistry data

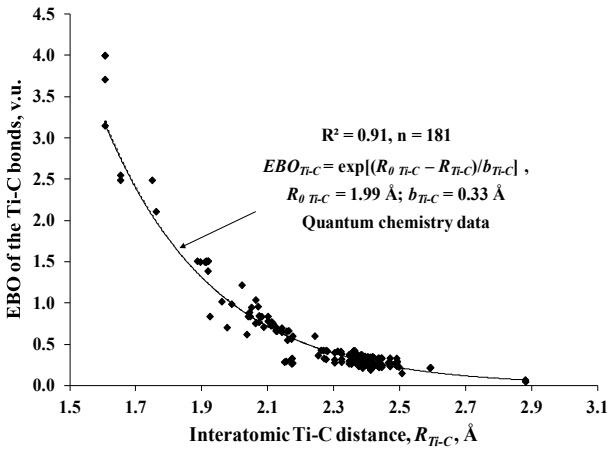

EBO and bond valence of the W-O bonds, v.u.
Interatomic W-O distance, R_{W-O}, Å
$s_{W-O} = \exp[(R_{0\ W-O} - R_{W-O})/b_{W-O}]$,
$R_{0\ W-O}$ = 1.896 Å; b_{W-O} = 0.28 Å
Crystal chemistry data
R² = 0.97, n = 72
$EBO_{W-O} = \exp[(R_{0\ W-O} - R_{W-O})/b_{W-O}]$,
$R_{0\ W-O}$ = 1.895 Å; b_{W-O} = 0.29 Å
Quantum chemistry data

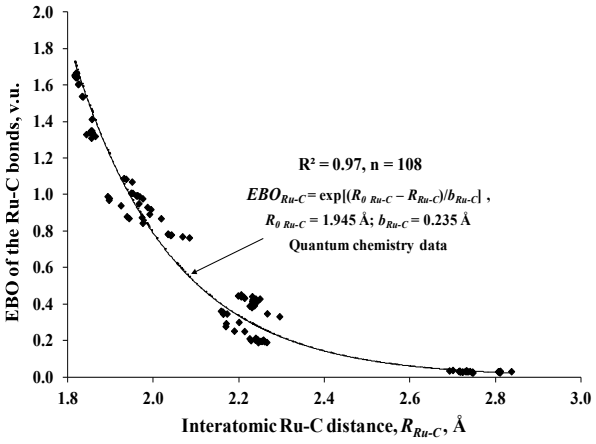

EBO and bond valence of the U-O bonds, v.u.
Interatomic U-O distance, R_{U-O}, Å
R² = 0.97, n = 325
$EBO_{U-O} = \exp[(R_{0\ U-O} - R_{U-O})/b_{U-O}]$,
$R_{0\ U-O}$ = 2.10 Å; b_{U-O} = 0.42 Å
Quantum chemistry data
$s_{U-O} = \exp[(R_{0\ U-O} - R_{U-O})/b_{U-O}]$,
$R_{0\ U-O}$ = 2.08 Å; b_{U-O} = 0.37 Å
Crystal chemistry data

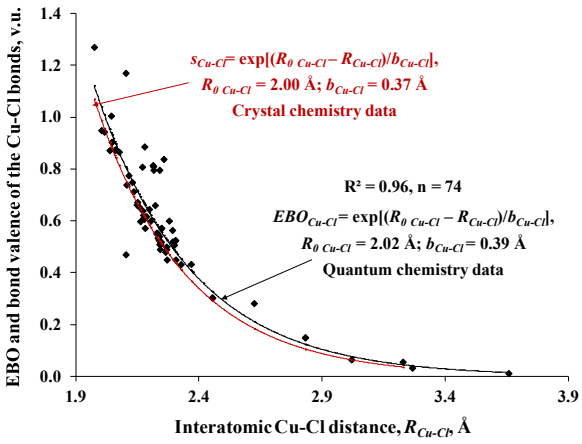

EBO and bond valence of the Ti-N bonds, v.u.
Interatomic Ti-N distance, R_{Ti-N}, Å
$s_{Ti-N} = \exp[(R_{0\ Ti-N} - R_{Ti-N})/b_{Ti-N}]$,
$R_{0\ Ti-N}$ = 1.906 Å; b_{Ti-N} = 0.37 Å
Crystal chemistry data
R² = 0.97, n = 92
$EBO_{Ti-N} = \exp[(R_{0\ Ti-N} - R_{Ti-N})/b_{Ti-N}]$,
$R_{0\ Ti-N}$ = 1.885 Å; b_{Ti-N} = 0.315 Å
Quantum chemistry data

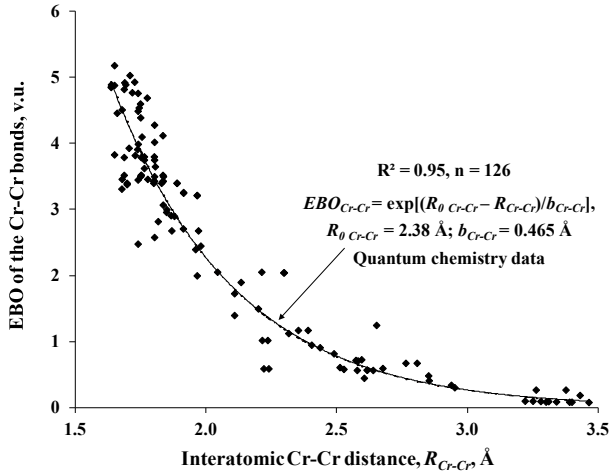

EBO and bond valence of the Fe-N bonds, v.u.
Interatomic Fe-N distance, R_{Fe-N}, Å
R² = 0.96, n =110
$EBO_{Fe-N} = \exp[(R_{0\ Fe-N} - R_{Fe-N})/b_{Fe-N}]$,
$R_{0\ Fe-N}$ = 1.812 Å; b_{Fe-N} = 0.345 Å
Quantum chemistry data
$s_{Fe-N} = \exp[(R_{0\ Fe-N} - R_{Fe-N})/b_{Fe-N}]$,
$R_{0\ Fe-N}$ = 1.815 Å; b_{Fe-N} = 0.37 Å
Crystal chemistry data

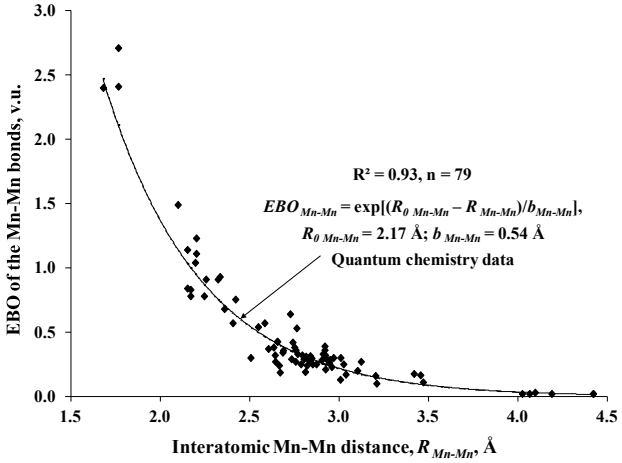

EBO and bond valence of the U-N bonds, v.u.
Interatomic U-N distance, R_{U-N}, Å
$s_{U-N} = \exp[(R_{0\ U-N} - R_{U-N})/b_{U-N}]$,
$R_{0\ U-N}$ = 2.24 Å; b_{U-N} = 0.37 Å
Crystal chemistry data
R² = 0.94, n = 155
$EBO_{U-N} = \exp[(R_{0\ U-N} - R_{U-N})/b_{U-N}]$,
$R_{0\ U-N}$ = 2.218 Å; b_{U-N} = 0.388 Å
Quantum chemistry data

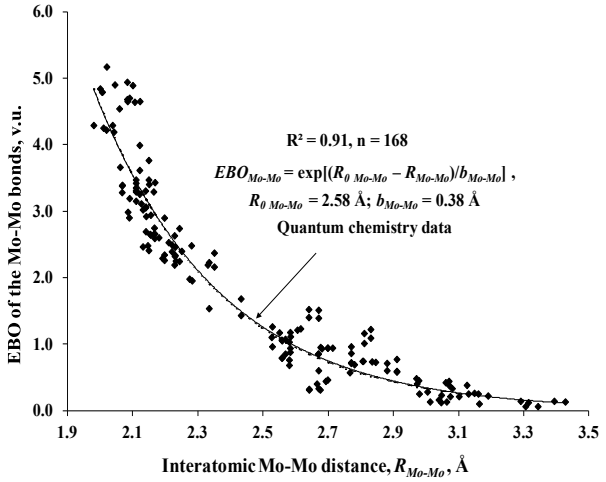

EBO of the Ti-C bonds, v.u.
Interatomic Ti-C distance, R_{Ti-C}, Å
R² = 0.91, n = 181
$EBO_{Ti-C} = \exp[(R_{0\ Ti-C} - R_{Ti-C})/b_{Ti-C}]$,
$R_{0\ Ti-C}$ = 1.99 Å; b_{Ti-C} = 0.33 Å
Quantum chemistry data

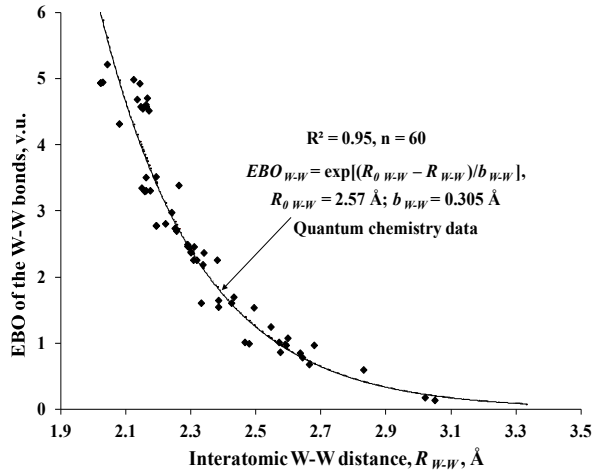

EBO of the Ru-C bonds, v.u.
Interatomic Ru-C distance, R_{Ru-C}, Å
R² = 0.97, n = 108
$EBO_{Ru-C} = \exp[(R_{0\ Ru-C} - R_{Ru-C})/b_{Ru-C}]$,
$R_{0\ Ru-C}$ = 1.945 Å; b_{Ru-C} = 0.235 Å
Quantum chemistry data


EBO and bond valence of the Cu-Cl bonds, v.u.
Interatomic Cu-Cl distance, R_{Cu-Cl}, Å
$s_{Cu-Cl} = \exp[(R_{0\ Cu-Cl} - R_{Cu-Cl})/b_{Cu-Cl}]$,
$R_{0\ Cu-Cl}$ = 2.00 Å; b_{Cu-Cl} = 0.37 Å
Crystal chemistry data
R² = 0.96, n = 74
$EBO_{Cu-Cl} = \exp[(R_{0\ Cu-Cl} - R_{Cu-Cl})/b_{Cu-Cl}]$,
$R_{0\ Cu-Cl}$ = 2.02 Å; b_{Cu-Cl} = 0.39 Å
Quantum chemistry data


EBO of the Cr-Cr bonds, v.u.
Interatomic Cr-Cr distance, R_{Cr-Cr}, Å
R^2 = 0.95, n = 126
$EBO_{Cr-Cr} = \exp[(R_{0\ Cr-Cr} - R_{Cr-Cr})/b_{Cr-Cr}]$,
$R_{0\ Cr-Cr}$ = 2.38 Å; b_{Cr-Cr} = 0.465 Å
Quantum chemistry data


EBO of the Mn-Mn bonds, v.u.
Interatomic Mn-Mn distance, R_{Mn-Mn}, Å
R^2 = 0.93, n = 79
$EBO_{Mn-Mn} = \exp[(R_{0\ Mn-Mn} - R_{Mn-Mn})/b_{Mn-Mn}]$,
$R_{0\ Mn-Mn}$ = 2.17 Å; b_{Mn-Mn} = 0.54 Å
Quantum chemistry data


EBO of the Mo-Mo bonds, v.u.
Interatomic Mo-Mo distance, R_{Mo-Mo}, Å
R^2 = 0.91, n = 168
$EBO_{Mo-Mo} = \exp[(R_{0\ Mo-Mo} - R_{Mo-Mo})/b_{Mo-Mo}]$,
$R_{0\ Mo-Mo}$ = 2.58 Å; b_{Mo-Mo} = 0.38 Å
Quantum chemistry data


EBO of the W-W bonds, v.u.
Interatomic W-W distance, R_{W-W}, Å
R^2 = 0.95, n = 60
$EBO_{W-W} = \exp[(R_{0\ W-W} - R_{W-W})/b_{W-W}]$,
$R_{0\ W-W}$ = 2.57 Å; b_{W-W} = 0.305 Å
Quantum chemistry data

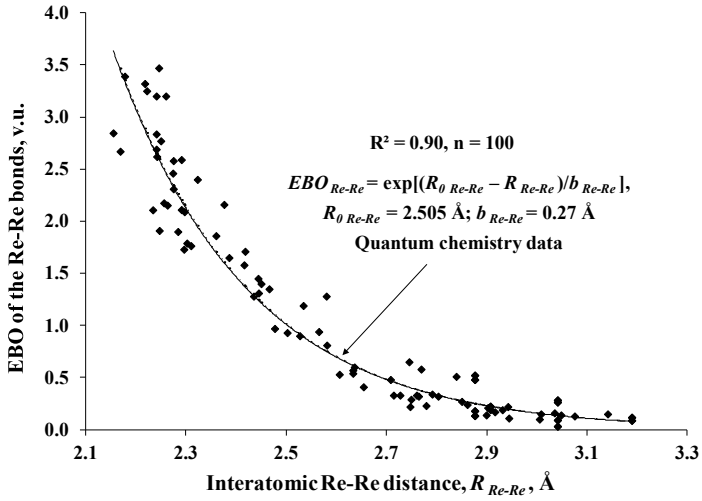

EBO of the Re-Re bonds, v.u.
Interatomic Re-Re distance, R_{Re-Re}, Å
R^2 = 0.90, n = 100
$EBO_{Re-Re} = \exp[(R_{0\ Re-Re} - R_{Re-Re})/b_{Re-Re}]$,
$R_{0\ Re-Re}$ = 2.505 Å; b_{Re-Re} = 0.27 Å
Quantum chemistry data

Figure S4. Correlation between the *BO* parameter $R_{0\ ij}$ and electron density constant *Cij*.

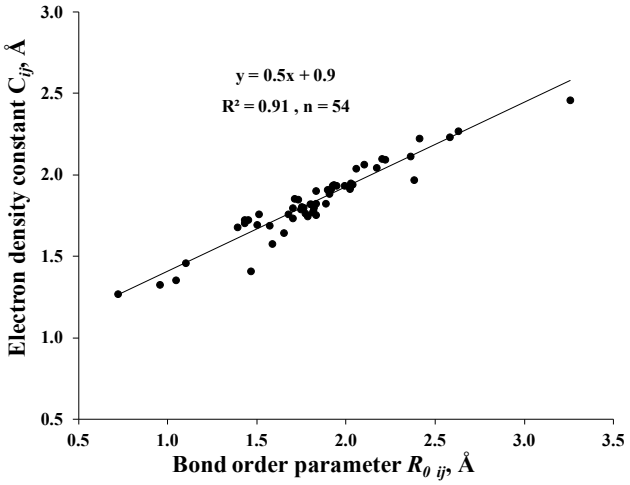


Figure S5. Bond order parameter $R_{0\ ij}$ (A) and electron density constant *Cij* (B) *vs*. the sum of the covalent radii of *i* and j atoms.

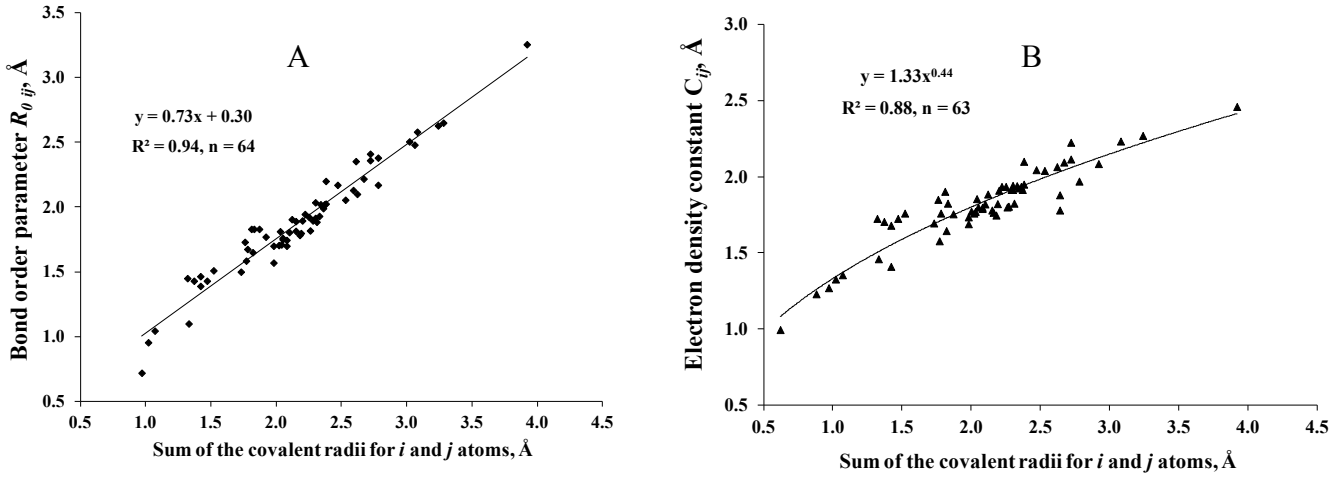


Figure S6. Relationship between electron density and bond order for some atom pairs.

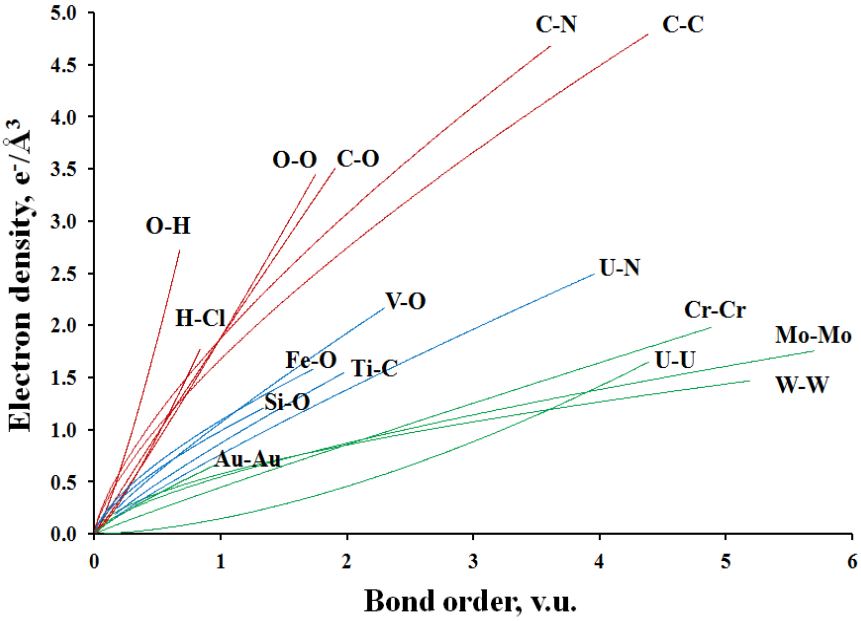
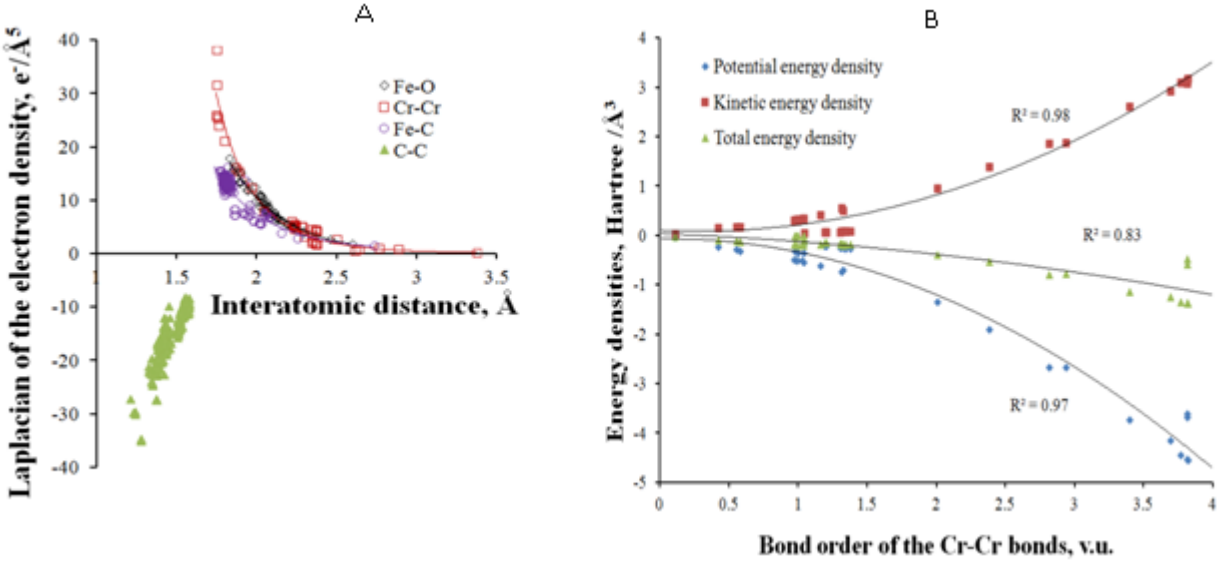


Figure S7. Additional parameters of the ED topology, which are not related to the Pauling's principles. A - Laplacian of the electron density as a function of the interatomic distance for the C-C, Fe-C, Cr-Cr and Fe-O bonds. B - Energy densities of the Cr-Cr bonds as a function of their *BOs*.



These parameters are widely used to describe the differences in the nature of chemical bonds. For example, as can be seen in Fig. S7A, in contrast to ionic or mixed ionic/covalent interactions, the Laplacian of the pure covalent C-C bonds is clearly negative. The key parameter to define the bond character is then the ratio between absolute value of the potential and kinetic energy

densities at the bond critical point [2], which is in turn related to the Laplacian value at this same position by the local expression of the quantum virial theorem [3]. For the ionic bonds this ratio is smaller then 1 (Laplacian >0), for the pure covalent bonds the ratio is larger than 2 (Laplacian <0), while the mixed interactions have the ratio between 1 and 2 (Laplacian >0). According to this parameter, the Cr-Cr interactions can be characterized as mixed ionic/covalent ones (Fig. S7B).

Figure S8. Linear correlation between the *BOs* of the Mo-O bonds calculated by Eq. 1 and the square of the stretching frequencies of various molybdates obtained in Raman spectroscopy. (The interatomic distances and stretching frequencies are taken from ref.[4])

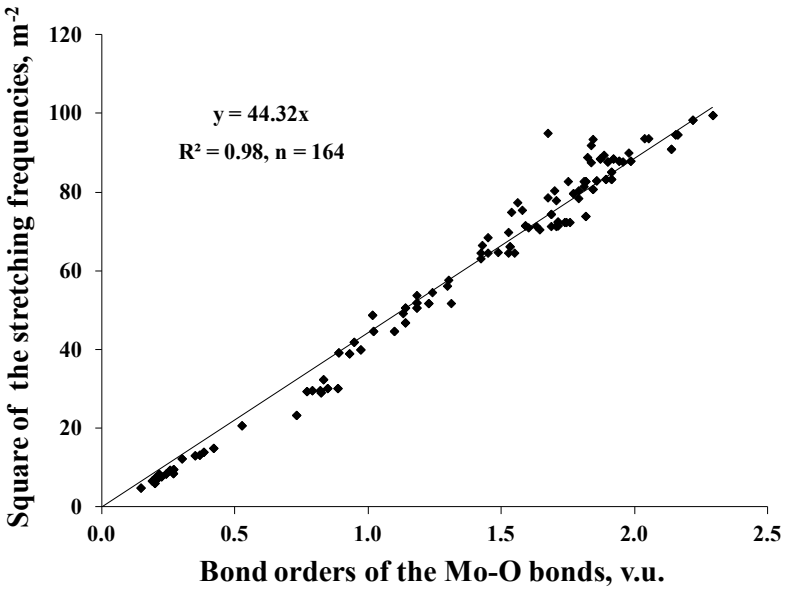


Table S1. The results of the exponential fitting of the quantum chemistry data by Eqs 1 and 3: Bond valence parameters and electron density constants for typical atomic pairs. *n* is a number of data points.

N	Bond	Bond valence parameters, Å		Quality of exponential fitting		Electron density constants, e/Å^3		Quality of exponential fitting		Ref.
		$R_{0\,ij}$	b_{ij}	R^2	n	C_{ij}	D_{ij}	R^2	n	
1	H-H					0.995	0.44	0.99	246	[5]
2	H-F					1.23	0.39	0.97	268	[2b, 5b, 5o, 6]
3	O-H	0.72	0.46	0.96	187	1.27	0.37	0.98	427	[5b, 5f, 7]
4	N-H	0.955	0.41	0.96	126	1.327	0.415	0.97	318	[5b, 5e, 7a, 7e, 7g, 7k, 7m, 7p, 7r-u, 7x, 7ae, 8]
5	C-H	1.045	0.365	0.98	75	1.355	0.435	0.99	398	[5b, 5d-f, 5o, 7s, 8a, 8b, 8i, 9]
6	Si-H	1.465	0.325	0.97	230	1.41	0.475	0.98	147	[8u, 10]
7	H-Cl	1.10	0.56	0.93	125	1.46	0.455	0.98	198	[5m, 6b, 6d, 7m, 7s, 8n, 8p, 8s, 8u, 11]
8	C-O	1.39	0.445	0.96	257	1.68	0.46	0.99	345	[5b, 5d, 5f, 7h, 7i, 7s, 8a, 8e, 8i, 9b, 9e, 9f, 9j, 9m, 12]
9	N-O	1.43	0.37	0.86	240	1.705	0.40	1.00	187	[5b, 7g, 7w, 7z, 8j, 8u, 9d, 9l, 11r, 12z, 12ae, 13]
10	Si-O	1.585	0.365	0.90	103	1.578	0.535	0.99	212	[6e, 8p, 8u, 10f, 10q, 10u, 10v, 13l, 14]
11	P-O	1.50	0.345	0.98	105	1.695	0.515	0.98	165	[8j, 12s, 13l, 14k, 14v, 15]
12	O-O	1.45	0.47	0.92	83	1.725	0.435	0.99	136	[5b, 5d, 7j, 7ab, 13m, 14d, 16]
13	Si-N	1.65	0.375	0.97	170	1.645	0.515	0.98	216	[8q, 10q, 10t, 10u, 14e, 14i, 14j, 14o, 14u, 14w, 14y, 17]
14	N-C	1.43	0.335	0.97	200	1.725	0.47	1.00	287	[5b, 5d, 7g-i, 7s, 8a-g, 8i, 8j, 9b, 9d, 9i, 9l, 9o, 12k, 12n, 12r, 12t, 12aj, 12am, 13e, 13k, 13o-q, 16n, 17f, 17l, 18]
15	C-C	1.51	0.345	0.96	373	1.76	0.485	0.99	786	[5b-d, 5f, 7h, 7i, 7p, 7s, 8a, 8e, 8i, 9d-g, 9i-m, 12d, 12j, 12k, 12n, 12r, 12t, 12al, 18c, 18e-g, 18x, 19]
16	Si-C	1.83	0.37	0.90	263	1.755	0.495	0.96	185	[10f, 10i, 10o, 10p, 10u-w, 10z, 14a, 14f, 14i, 14j, 17j, 17p, 17t,

										18p, 19o, 20]
17	N-Cl	1.71	0.585	0.93	66	1.855	0.455	0.98	124	[11d, 11n, 11r, 13m, 21]
18	N-P	1.675	0.335	0.95	157	1.76	0.53	0.99	178	[8k, 8o, 12aj, 14i, 15c, 15e, 15l, 15p, 17g, 17m, 18m, 18t, 22]
19	N-S	1.73	0.415	0.94	128	1.85	0.475	0.99	147	[5d, 8b, 8j, 14i, 15e, 16j, 23]
20	C-P	1.83	0.38	0.94	178	1.825	0.58	0.94	225	[8j, 8k, 9g, 9i, 9m, 9o, 9q, 12n, 12o, 15l-o, 18j, 18m, 18t, 18v, 20ac, 22o, 22r, 24]
21	C-S	1.83	0.325	0.97	203	1.903	0.533	0.98	220	[5d, 5g, 7g, 7h, 8b, 8u, 12n, 12ac, 12al, 14k, 18g, 18i, 18l, 18s, 18v, 19m, 23k, 25]
22	Ti-O	1.818	0.29	0.93	141	1.80	0.385	0.95	51	[9g, 11f, 12g, 12s, 16p, 26]
23	V-O	1.798	0.315	0.96	192	1.822	0.37	0.99	253	[7i, 7w, 12ak, 13b, 16e, 16p, 23d, 26k, 27]
24	Cr-O	1.76	0.315	0.93	164	1.80	0.38	0.97	61	[16p, 26h, 26j, 26k, 28]
25	Mn-O	1.75	0.34	0.95	53	1.805	0.38	0.99	71	[12t, 16p, 26h, 26k, 29]
26	Fe-O	1.783	0.387	0.95	77	1.747	0.41	0.94	156	[12m, 16p, 26h, 28i, 28l, 29b, 29f, 29n, 30]
27	Co-O	1.77	0.315	0.97	42	1.765	0.385	0.96	99	[7u, 13w, 16p, 26k, 29c, 29f, 30ı, 30n, 31]
28	Cu-O	1.57	0.47	0.87	149	1.69	0.47	0.97	185	[7u, 9d, 12t, 16a, 16b, 16p, 26k, 27g, 29b, 29h, 31c, 32]
29	Nb-O	1.915	0.295	0.98	89	1.915	0.39	0.95	34	[19l, 26k, 27a, 27h, 33]
30	Mo-O	1.895	0.27	0.96	95	1.91	0.37	0.99	58	[12x, 15a, 26k, 27a, 28h, 33c, 34]
31	Ru-O	1.905	0.355	0.95	46	1.885	0.39	0.98	104	[26k, 30k, 34c, 35]
32	W-O	1.895	0.29	0.97	72					[26j, 26k, 27a, 28l, 33c, 34h, 34m, 36]
33	U-O	2.10	0.42	0.97	325	2.065	0.42	0.97	151	[8b, 25e, 26l, 27a, 37]
34	Pu-O	2.055	0.385	0.98	38	2.04	0.39	0.99	34	[7f, 37m, 37q, 37v, 37aa, 38]
35	Ti-N	1.885	0.315	0.97	92	1.825	0.47	0.98	86	[26ı-k, 39]
36	Cr-N	1.805	0.285	0.92	109	1.82	0.42	0.97	93	[26j, 26k, 28e, 28g, 28l, 40]
37	Fe-N	1.812	0.345	0.96	110	1.771	0.45	0.96	83	[13c, 13d, 13u, 26k, 30d, 30g, 30i, 30k, 30o, 30p, 41]

38	Co-N					1.76	0.46	0.95	139	[12j, 19k, 26k, 28l, 30i, 31b-e, 31i-l, 40f, 41n, 42]
39	Cu-N	1.70	0.395	0.94	134	1.735	0.475	0.91	158	[9d, 12t, 18c, 18h, 29h, 31c, 32g, 32h, 32m, 32r-u, 32z, 32ac-ah, 32ak-am, 34c, 40f, 41n, 43]
40	Mo-N	1.923	0.325	0.92	116	1.935	0.43	0.99	69	[12x, 12z, 19c, 26j, 26k, 34c, 34g, 34l, 36a, 44]
41	W-N	1.93	0.275	0.95	140	1.94	0.43	0.98	53	[12ag, 18b, 23f, 26k, 36a, 44f, 45]
42	U-N	2.218	0.388	0.94	155	2.095	0.45	0.99	72	[8b, 8g, 37f, 37h, 37n-q, 37w, 37x, 37ac, 37ad, 46]
43	Ti-C	1.99	0.33	0.91	181	1.935	0.39	0.95	96	[9a, 9g, 9h, 11f, 12g, 19i, 19p, 26e, 26i, 26j, 37n, 39c, 39e, 47]
44	Cr-C	1.89	0.345	0.90	157					[9a, 12d, 12f, 12j, 12w, 12aa, 12ah, 19e, 19f, 26j, 28g, 40e, 47a, 48]
45	Mn-C	1.815	0.315	0.95	47	1.78	0.485	0.94	126	[9j, 9k, 9m, 12i, 12u, 12x, 19f, 19l, 47a, 49]
46	Fe-C	1.745	0.36	0.90	146	1.79	0.53	0.95	188	[9c, 9k, 12d, 12f, 12h, 12i, 12m, 12aa, 19f, 22b, 41i, 47a, 47b, 47g, 47j, 48f, 50]
47	Co-C	1.705	0.46	0.89	70					[9f, 12c, 12d, 31e, 42i, 47a, 47i, 47j, 49d, 50g, 51]
48	Ni-C					1.773	0.48	0.97	77	[10i, 12aa, 48f, 52]
49	Cu-C	1.70	0.347	0.82	122	1.798	0.46	0.98	42	[12d, 18c, 18d, 32ac, 43b, 43d, 43h, 43m, 48i, 49d, 53]
50	Mo-C	2.035	0.365	0.94	109	1.942	0.50	0.96	62	[12v-z, 12ah, 19c, 26j, 34b, 44e, 47g, 48g, 54]
51	Ru-C	1.945	0.235	0.97	108	1.935	0.45	0.93	95	[12ab, 22b, 35c, 49e, 55]
52	W-C	2.025	0.29	0.91	230	1.95	0.465	0.92	85	[12ag, 12ah, 26j, 28g, 36b, 45c, 48g, 50c, 54f, 54l, 54m, 55f, 56]
53	U-C	2.36	0.475	0.91	162	2.115	0.46	0.88	52	[37c, 37n, 46g, 46h, 46k, 46q, 47c, 54b, 57]
54	Cu-Cl	2.02	0.39	0.96	74	1.925	0.465	0.98	85	[32ag, 43f, 43h, 43k, 53j, 58]
55	Ag-Cl	2.17	0.43	0.96	41	2.045	0.475	0.99	41	[53j, 58b, 58d]
56	Au-Cl	2.20	0.42	0.97	55	2.10	0.52	1.00	53	[11q, 53j, 58b, 58d, 58e, 59]
57	Fe-P	2.13	0.485	0.90	41					[9c, 12i, 12w, 22b, 41b, 41d, 41g, 50i, 50m, 50n, 60]

58	Mo-P	2.353	0.29	0.93	52					[12v-z, 15a, 44b, 44g, 54c, 54j, 61]
59	Ni-S					1.915	0.55	0.91	43	[25i, 28l, 52d, 62]
60	Cu-S	2.02	0.38	0.92	47	1.915	0.53	0.99	106	[18h, 32ah, 40f, 58a, 63]
61	V-V	2.48	0.395	0.93	61					[49d, 64]
62	Cr-Cr	2.38	0.465	0.95	126	1.97	0.49	0.91	38	[40c, 48g, 49d, 64e-g, 65]
63	Mn-Mn	2.17	0.54	0.93	79					[9j, 12i, 12q, 12u, 49a, 49b, 49d, 64e, 64f, 65i, 65w, 65ac, 66]
64	Fe-Fe					1.88	0.60	0.97	41	[12h, 12i, 13d, 49b, 49d, 50j, 64e-g, 65a, 65i, 66f, 67]
65	Cu-Cu					1.78	0.525	0.96	116	[32f, 32k, 32z, 49d, 53e, 58b-d, 59c, 63f, 68]
66	Nb-Nb	2.65	0.408	0.88	41					[49d, 64g, 64h, 67c, 69]
67	Mo-Mo	2.58	0.38	0.91	168	2.233	0.575	0.99	72	[12v, 12y, 34c, 34e, 34f, 34j, 34l, 34o, 48g, 49d, 54c, 54n, 54o, 61, 64g, 65m, 65n, 65p, 65v, 65z, 67c, 69b, 70]
68	Ru-Ru					2.085	0.58	0.96	43	[34c, 49d, 55a, 55c, 55h, 65b, 67c, 69b, 71]
69	W-W	2.628	0.375	0.96	81	2.27	0.65	0.99	18	[12ag, 36c, 48g, 56e, 56h, 64g, 65n, 65v, 65z, 70c, 70e, 70k, 70l, 70v, 72]
70	Re-Re	2.505	0.27	0.90	100					[48g, 65n, 65r, 70s, 70v, 73]
71	Au-Au	2.41	0.41	0.91	49	2.225	0.49	0.97	79	[42k, 53n, 58b, 58d, 59c, 59d, 68h, 74]
72	U-U	3.255	0.658	0.86	95	2.46	0.44	0.96	25	[37e, 37g, 46r, 57d, 65z, 70k, 75]

Table S2. The results of the *BO* calculations for the Re_6-cluster complexes.

N	Compound	VEC*	Bond length, Å			Bond order, v.u.			Total electron count for Re, v.u.		Cryst. Struct. ref.
			Re-Re	Re-L^i	Re-L^a	Re-Re	Re-L^i	Re-L^a	Expect	Calcul	
1	$[Bu_4N][Re_6S_8Cl_4(py)_2]$	23	2.596	2.401	N: 2.161 Cl: 2.400	0.68	0.92	N: 0.58 Cl: 0.60	7	7.00	[76]
2	$[Ph_4P]_3[Re_6S_8(CN)_6]$	23	2.606	2.411	2.150	0.66	0.89	0.65	7	6.87	[77]
3	$Cs_6Re_6S_{15}$	24	2.605	2.403	2.451	0.66	0.92	0.80	7	7.10	[78]
4	$[Bu_4N]_4[Re_6S_8Br_6]$	24	2.592	2.395	2.595	0.69	0.94	0.68	7	7.19	[79]
5	$[Bu_4N]_4[Re_6S_8I_6]$	24	2.598	2.403	2.787	0.68	0.92	0.62	7	7.00	[79]
6	$[Re_6S_8(PEt_3)_4(Br)_2]$	24	2.599	2.404	P: 2.466 Br: 2.550	0.67	0.91	P: 0.98 Br: 0.76	7	7.26	[80]
7	$[Re_6S_8(PEt_3)_6]Br_2*CH_2Cl_2$	24	2.614	2.405	2.483	0.64	0.91	0.94	7	7.13	[80]
8	$Cs_3Na[Re_6S_8(CN)_6]$	24	2.602	2.411	2.119	0.67	0.90	0.71	7	6.97	[81]
9	$[Ph_4P]_4[Re_6S_8(CN)_6]*(CH_3CN)_2$	24	2.608	2.404	2.166	0.65	0.91	0.62	7	6.88	[82]
10	$[Bu_4N]_4[Re_6S_8Cl_6]$	24	2.603	2.404	2.450	0.66	0.91	0.55	7	6.86	[79]
11	$[Bu_4N]_2[Re_6S_8Cl_4(cpy)_2]$	24	2.593	2.400	N: 2.212 Cl: 2.423	0.69	0.92	N: 0.53 Cl: 0.59	7	7.03	[76]
12	$[Bu_4N][Re_6S_8Cl_3(py)_3]$	24	2.594	2.401	N: 2.187 Cl: 2.424	0.69	0.92	N: 0.57 Cl: 0.59	7	7.02	[76]
13	$[Bu_4N]_2[Re_6S_8Cl_4(ppy)_2]$	24	2.598	2.410	N: 2.216 Cl: 2.435	0.68	0.90	N: 0.53 Cl: 0.57	7	6.86	[83]
14	$Cs_6Re_6Se_{15}$	24	2.634	2.523	2.574	0.59	0.94	0.82	7	6.95	[84]
15	$Re_6Se_8(PEt_3)_4(I)_2*2CHCl_3$	24	2.641	2.521	P: 2.481 I: 2.747	0.58	0.94	P: 0.95 I: 0.69	7	6.94	[85]
16	$Re_6Se_8(PEt_3)_4(CN)_2$	24	2.647	2.522	P: 2.478 C: 2.104	0.56	0.94	P: 0.95 C: 0.75	7	6.91	[86]
17	$[Re_6Se_8(PEt_3)_4(CO)_2][SbF_6]_2$	24	2.640	2.518	P: 2.484 C: 2.060	0.58	0.95	P: 0.94 C: 0.85	7	7.04	[87]
18	$Re_6Se_8(PEt_3)_5(CN)(BPh4)$	24	2.634	2.509	P: 2.478 C: 2.143	0.59	0.98	P: 0.95 C: 0.67	7	7.18	[86]
19	Re_6Te_{15}	24	2.676	2.692	2.710	0.51	1.02	0.98	7	7.09	[88]
20	$[Mn(salen)]_{4n}[Re_6Te_8(CN)_6]_n$	24	2.693	2.694	2.105	0.47	1.02	C: 0.75	7	6.71	[89]

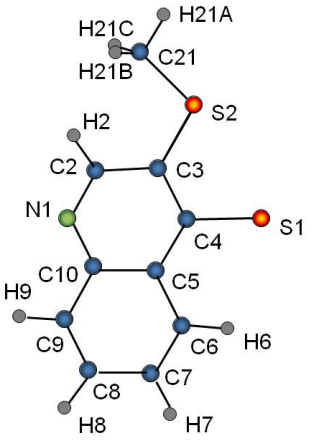
* VEC = the total number of valence electrons of the cluster.

Table S3. Bond valence parameters used in this work.

i-j pair	Bond valence parameter, Å	
	$R_{0\ ij}$	b_{ij}
Re-Re	2.495	0.265
Re-N	1.98	0.37
Re-C	2.007	0.335
Re-Cl	2.23	0.37
Re-S	2.37	0.37
Re-Br	2.45	0.37
Re-P	2.46	0.37
Re-Se	2.50	0.37
Re-I	2.61	0.37

12. Electron descriptors calculated by Eqs 1 and 3 (Examples)

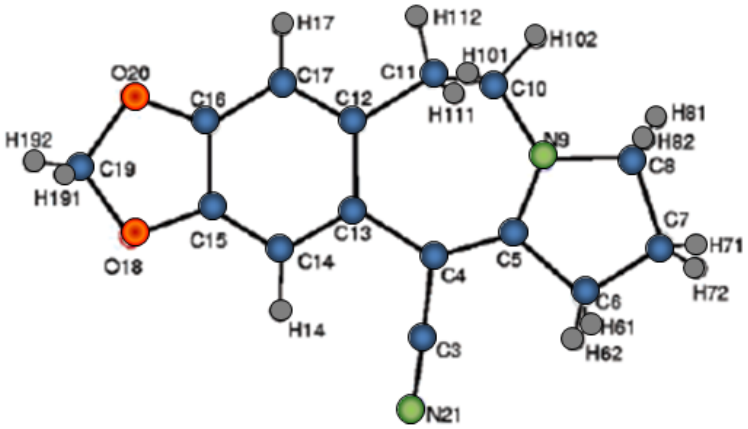
12.1. Electron density at the bond critical points in 4-[[4-(methoxy)-3-quinolinyl]thio]-3-thiomethylquinoline (See the fragment of the crystal structure).



Bond	R_{ij}, Å	ρ_c, e/Å^3 Eq. 3 This work	ρ_c, e/Å^3 Ref. [90]		Relative difference, %	
			Model I*	Model II**	This work - Model I	Model I – Model II
S1-C4	1.782	1.25	1.28	1.01	2.3	21.1
S1-C13	1.770	1.28	1.27	1.03	0.8	18.9
S2-C3	1.758	1.31	1.30	1.05	0.8	19.2
S2-C21	1.808	1.20	1.26	0.98	4.8	22.2
C2-C3	1.428	1.98	2.00	1.41	1.0	29.5
C3-C4	1.390	2.14	2.12	1.50	0.9	29.2
C4-C5	1.426	1.99	1.96	1.41	1.5	28.1
C5-C6	1.421	2.01	2.00	1.43	0.5	28.5
C6-C7	1.376	2.20	2.23	1.53	1.3	31.4
C7-C8	1.416	2.03	2.07	1.44	1.9	30.4
C8-C9	1.378	2.20	2.18	1.53	0.9	29.8
C9-C10	1.417	2.03	2.06	1.43	1.5	30.6
N1-C2	1.317	2.38	2.53	1.86	5.9	26.5
N1-C10	1.367	2.14	2.19	1.71	2.3	21.9
N11-C12	1.317	2.38	2.52	1.85	5.6	26.6
N11-C20	1.374	2.11	2.13	1.69	0.9	20.7
C21-H21A	1.068	1.93	1.73	1.29	11.6	25.4
C21-H21B	0.986	2.34	1.84	1.45	27.2	21.2
C21-H21C	0.995	2.29	1.85	1.44	23.8	22.2
C2-H2	1.081	1.88	1.87	1.24	0.5	33.7
C6-H6	1.072	1.92	1.85	1.26	3.8	31.9
C7-H7	1.080	1.88	1.76	1.24	6.8	29.5
C8-H8	1.079	1.89	1.72	1.24	9.9	27.9
C9-H9	1.083	1.87	1.75	1.24	6.9	29.1
O1…H22B	2.020	0.13	0.04	0.04	225.0	0
H6…H16	2.201	0.08	0.08	0.03	0	62.5
O1…O1	3.178	0.06	0.04	0.03	50.0	25.0

*Multipolar model.
**Independent Atom Model.

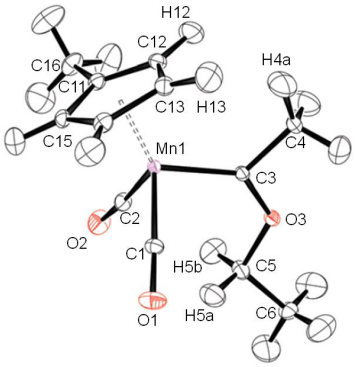
12.2. Electron density at the bond critical points in 5,8,9,10-Tetrahydro-6H-1,3-dioxolo[4,5-h]pyrrolo[2,1-b]-[3]benzazepine-11-carbonitrile



Bond	R_{ij}, Å	ρ_c, e/Å^3 Eq. 3 This work	ρ_c, e/Å^3 Ref. [91]	Relative difference, %
C19-O20	1.427	1.73	1.75	1.1
C19-O18	1.435	1.70	1.65	3.0
C16-O20	1.373	1.95	1.92	1.6
C15-O18	1.378	1.93	1.90	1.6
C15-C16	1.385	2.17	2.19	0.9
C17-C16	1.376	2.21	2.18	1..4
C14-C15	1.375	2.21	2.15	2.8
C14-C13	1.422	2.01	1.99	1.0
C17-C12	1.411	2.05	1.96	4.6
C13-C12	1.411	2.05	1.97	4.1
C12-C11	1.503	1.70	1.70	0
C4-C13	1.480	1.78	1.66	7.2
C4-C3	1.424	2.00	1.82	9.9
C4-C5	1.389	2.15	2.05	4.9
C10-C11	1.534	1.59	1.58	0.6
C6-C5	1.513	1.66	1.59	4.4
C6-C7	1.538	1.58	1.57	0.6
C8-C7	1.530	1.61	1.60	0.6
C3-N21	1.165	3.29	3.42	3.8
C10-N9	1.455	1.78	1.73	2.9
C8-N9	1.465	1.74	1.63	6.7
C5-N9	1.342	2.26	2.29	1.3

12.3. Electron density at the bond critical points in MeCp(CO)2Mn=C(OEt)Me.

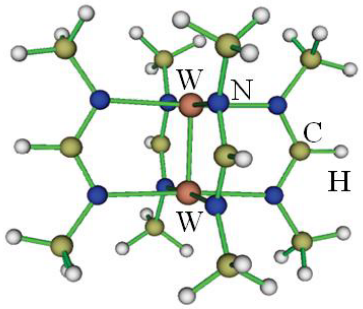
The first and the second rows are related to the experimental and theoretical data, respectively, of the original work.



Bond	R_{ij}, Å	ρ_c, e/Å^3 Eq. 3 This work	ρ_c, e/Å^3 Ref.[92]	Relative difference, %
Mn1-C1	1.784	0.99	1.03	3.9
	1.781	1.00	1.03	2.9
Mn1-C2	1.780	1.00	1.01	1.0
	1.776	1.01	1.04	2.9
Mn1-C3	1.901	0.78	0.99	21.2
	1.900	0.78	0.89	12.4
Mn1-C11	2.167	0.45	0.41	9.8
	2.169	0.45	0.50	10.0
Mn1-C12	2.153	0.46	0.50	8.0
Mn1-C13	2.160	0.46	0.41	12.2
	2.151	0.47	0.49	4.1
Mn1-C14	2.160	0.46	0.40	15.0
	2.145	0.47	0.52	9.6
Mn1-C15	2.157	0.46	0.49	6.1
C1-O1	1.161	3.09	3.47	11.0
	1.158	3.11	3.09	0.6
C2-O2	1.164	3.07	3.49	12.0
	1.160	3.10	3.07	1.0
C3-C4	1.516	1.43	1.69	15.4
	1.508	1.45	1.78	18.5
C3-O3	1.334	2.12	2.15	1.4
	1.331	2.14	2.01	6.5
C5-O3	1.442	1.68	1.64	2.4
	1.436	1.70	1.63	4.3
C5-C6	1.508	1.68	1.77	5.1
	1.502	1.70	1.78	4.5
C11-C12	1.424	2.00	2.09	4.3
	1.417	2.03	2.01	1.0
C11-C15	1.430	1.97	2.07	4.8
	1.425	2.00	1.98	1.0
C11-C16	1.498	1.72	1.75	1.7
	1.487	1.76	1.80	2.2
C12-C13	1.427	1.99	2.01	1.0
	1.418	2.02	1.99	1.5
C13-C14	1.422	2.01	2.00	0.5
	1.417	2.03	2.00	1.5
C14-C15	1.420	2.02	2.04	1.0
	1.412	2.05	2.02	1.5

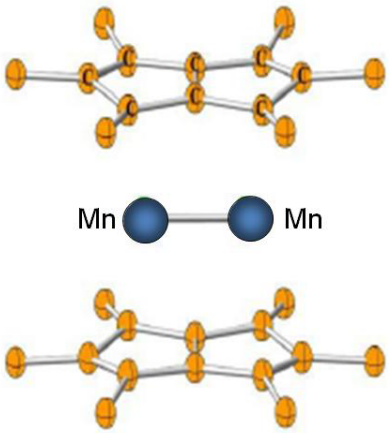
C12-H12a	1.083	1.87	1.82	2.7
	1.078	1.89	1.95	3.1
C13-H13a	1.083	1.87	1.86	0.5
	1.077	1.89	1.95	3.1
C14-H14a	1.083	1.87	1.85	1.1
	1.077	1.89	1.96	3.6
C15-H15a	1.083	1.87	1.87	0
	1.078	1.89	1.95	3.1
C16-H16a	1.093	1.83	1.78	2.8
	1.087	1.85	1.90	2.6
C16-H16b	1.093	1.83	1.76	4.0
	1.091	1.83	1.88	2.7
C16-H16c	1.093	1.83	1.74	5.2
	1.088	1.85	1.91	3.1
C1-H5a	2.410	0.09	0.08	12.5
	2.422	0.09	0.08	12.5
C2-H5b	2.530	0.07	0.09	22.2
	2.515	0.07	0.08	12.5
O1-H4a_4	2.520	0.03	0.02	50.0
O2-H5b_3	2.600	0.03	0.03	0
O2-H5a_3	2.515	0.03	0.02	50.0
H4a-O1_4	2.520	0.03	0.02	50.0
H5b-O2_3	2.600	0.03	0.03	0
H15a-O2_1	2.515	0.03	0.02	50.0
H4a-H12a	2.35	0.05	0.05	0
H4a-H13a	2.14	0.07	0.04	75.0
H4c-H6a_4	2.24	0.06	0.02	200.0
H5a-H12a_4	2.558	0.03	0.03	0
H6a-H4c_4	2.24	0.06	0.01	500.0
H6b-H15a_1	2.347	0.05	0.03	66.7
H6c-H13a_3	2.344	0.05	0.01	400.0
H16a-H16b_2	2.478	0.03	0.02	50.0
H16b-H16a_2	2.478	0.03	0.02	50.0
H13a-H6c_3	2.344	0.05	0.01	400.0
H15a-H6b_1	2.347	0.05	0.03	66.7

12.4. Bond orders in the W_2^{6+} paddlewheel complex.



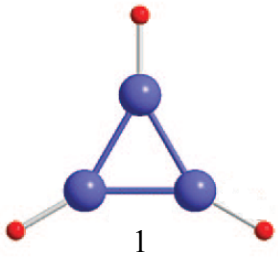
Bond	R_{ij}, Å	*BO*, v.u. Eq. 1 This work	Wiberg *BO*, v.u. Ref.[12ag]	Relative difference, %
W-W	2.175	3.35	3.31	1.2
W-N	2.131	0.48	0.53	9.4

12.5. Bond orders in $Mn_2C_8Me_6$.



Bond	R_{ij}, Å	*BO*, v.u. Eq. 1 This work	*BO*, v.u. Ref.[49d]		Relative difference, %	
			DI	Wiberg	This work-Wiberg	Wiberg-DI
Mn1-Mn2	2.202	0.94	1.11	1.23	23.6	9.8
Mn1-C1	2.053	0.47	0.50	0.64	26.6	21.9
Mn1-C2	2.060	0.46	0.42	0.58	20.7	27.6
Mn1-C3	2.053	0.47	0.50	0.64	26.6	21.9
Mn1-C4	2.161	0.33	0.29	0.40	12.1	21.2
Mn1-C5	2.161	0.33	0.29	0.40	12.1	21.2

12.6. Bond orders in the planar uranium oxides.



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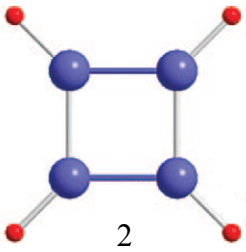

2

Balance of the valence electrons:
The sum of valence electrons for U atom should be equal to 8:
6 (uranium electrons) + 2 (oxygen electrons)
Each U is bonded to oxygen atom and two other U atoms. The sum of bond orders for the three bonds should be equal to 8 v.u.

N	Compound	Bond	R_{ij}, Å	*BO*, v.u. Eq. 1 This work	Discrepancy in the number of valence electrons, v.u.	Wiberg Bond Index, v.u. Ref. [93]	Discrepancy in the number of valence electrons, v.u.
1	cyclo-U_3O_3	U-U U-O	2.539 1.833	2.898 1.888		2.735 2.028	
		BVS		7.684	0.316	7.498	0.502
2	cyclo-U_4O_4	U-U U-O	2.539 1.830	2.898 1.902		2.478 2.059	
		BVS		7.698	0.302	7.015	0.985

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