Intermolecular carbonyl-carbonyl interactions in metal complexes

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SUPPORTING INFORMATION

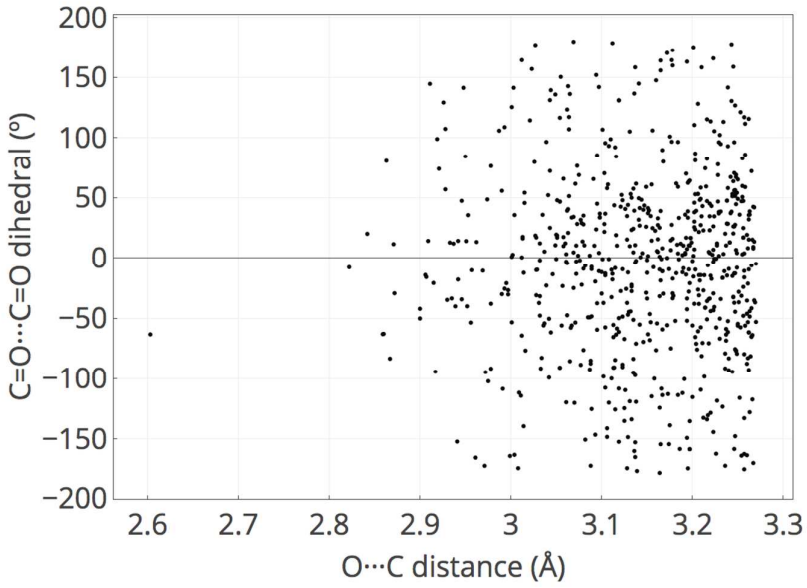


Figure S1. C=O···C=O dihedral as a function of the intermolecular O···C distance in crystal structures with short R-CO···CO contacts.

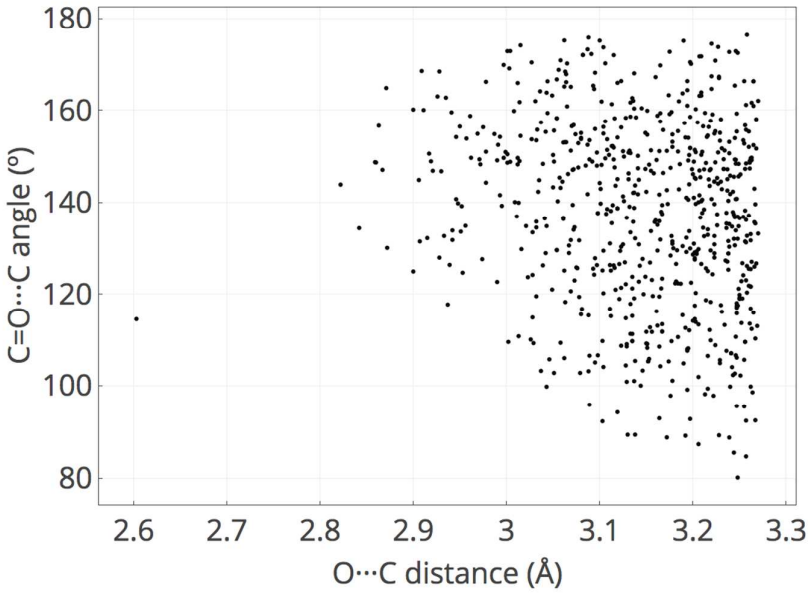
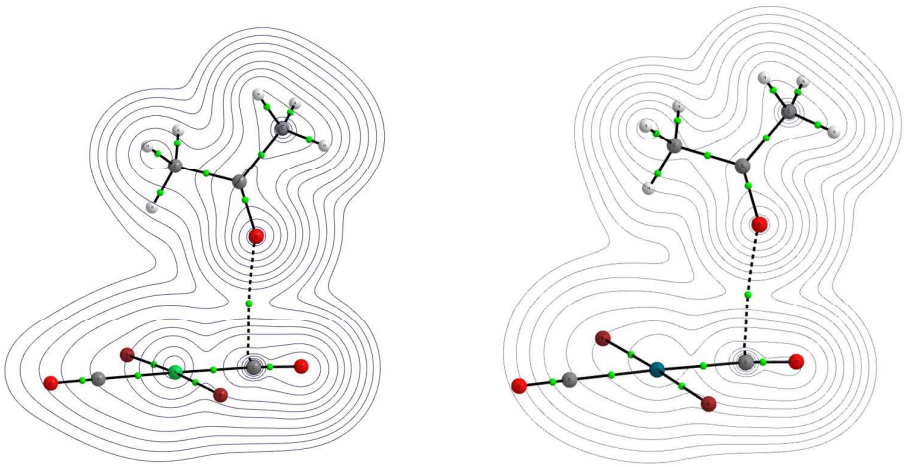
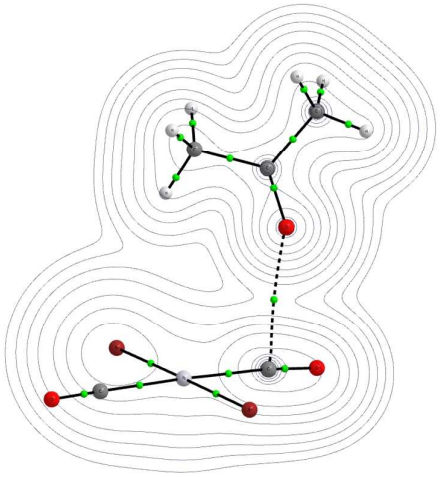


Figure S2. C=O···C angle as a function of the intermolecular O···C distance in crystal structures with short R-CO···CO contacts.



Ni Pd



Pt

Figure S3. O···C bond paths and associated BCPS and 2D electron density contours on the plane defined by the two atoms and the BCP involved in the O···C=O contact for the three [*trans*-$MBr_2(CO)_2$] (M = Ni, Pd, Pt) complexes.

Table 1. Cartesian coordinates of the optimized structures of [*trans*-$MBr_2(CO)_2$] (M = Ni, Pd, Pt) complexes.

Ni

Br	2.379787	1.329317	-0.028041
Ni	0.750574	-0.317021	0.134160
C	1.406569	-1.069929	-1.397916
Br	-0.772333	-2.070103	0.318801
C	0.122979	0.450012	1.693137
O	-0.221671	0.894580	2.665268
O	-1.826875	1.637005	-0.077068
C	-2.937319	1.404616	-0.505446
C	-3.338246	1.798082	-1.907445
C	-3.975657	0.691579	0.327506
H	-3.715259	0.741709	1.382407
H	-4.975033	1.097500	0.162162
H	-3.994695	-0.360272	0.026120
H	-2.476636	2.172039	-2.455629
H	-3.780749	0.948458	-2.433348
H	-4.105247	2.576514	-1.862463
O	1.811133	-1.533836	-2.339620

Pd

Br	2.552737	1.299660	-0.167724
Pd	0.698765	-0.289272	0.162985
C	1.445376	-1.413960	-1.237936
Br	-1.101410	-1.950989	0.496013
C	-0.005945	0.844761	1.611988
O	-0.355170	1.468560	2.475676
O	-2.073097	1.814383	-0.149868
C	-3.094141	1.445760	-0.690069
C	-3.255535	1.496155	-2.191039
C	-4.255793	0.895991	0.102433
H	-4.138997	1.132481	1.157611
H	-5.209544	1.275525	-0.269129
H	-4.270356	-0.191802	-0.013827
H	-2.323118	1.800912	-2.660548
H	-3.567868	0.521364	-2.573828
H	-4.044161	2.207012	-2.452984
O	1.879596	-2.064780	-2.044179

Pt

Br	-0.127130	2.459189	0.335279
Pt	0.682617	0.116618	0.107666
C	1.788517	0.648348	-1.380459
Br	1.511966	-2.213139	-0.124645
C	-0.379459	-0.419450	1.662200
O	-0.922538	-0.716779	2.598738
O	-2.795508	-0.967687	0.254018
C	-3.688323	-0.694470	-0.519356
C	-3.638796	0.536653	-1.392400
C	-4.906093	-1.579593	-0.653840
H	-4.769560	-2.496451	-0.085202
H	-5.785691	-1.048087	-0.279634
H	-5.100606	-1.813373	-1.703205
H	-2.817605	1.184000	-1.093208
H	-3.498537	0.232276	-2.433964
H	-4.584022	1.082343	-1.348287
O	2.441492	0.959762	-2.243193