Electronic Supplementary Information

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Electrocatalytic reduction of CO_2 to CO by a mononuclear Ru(II) complex

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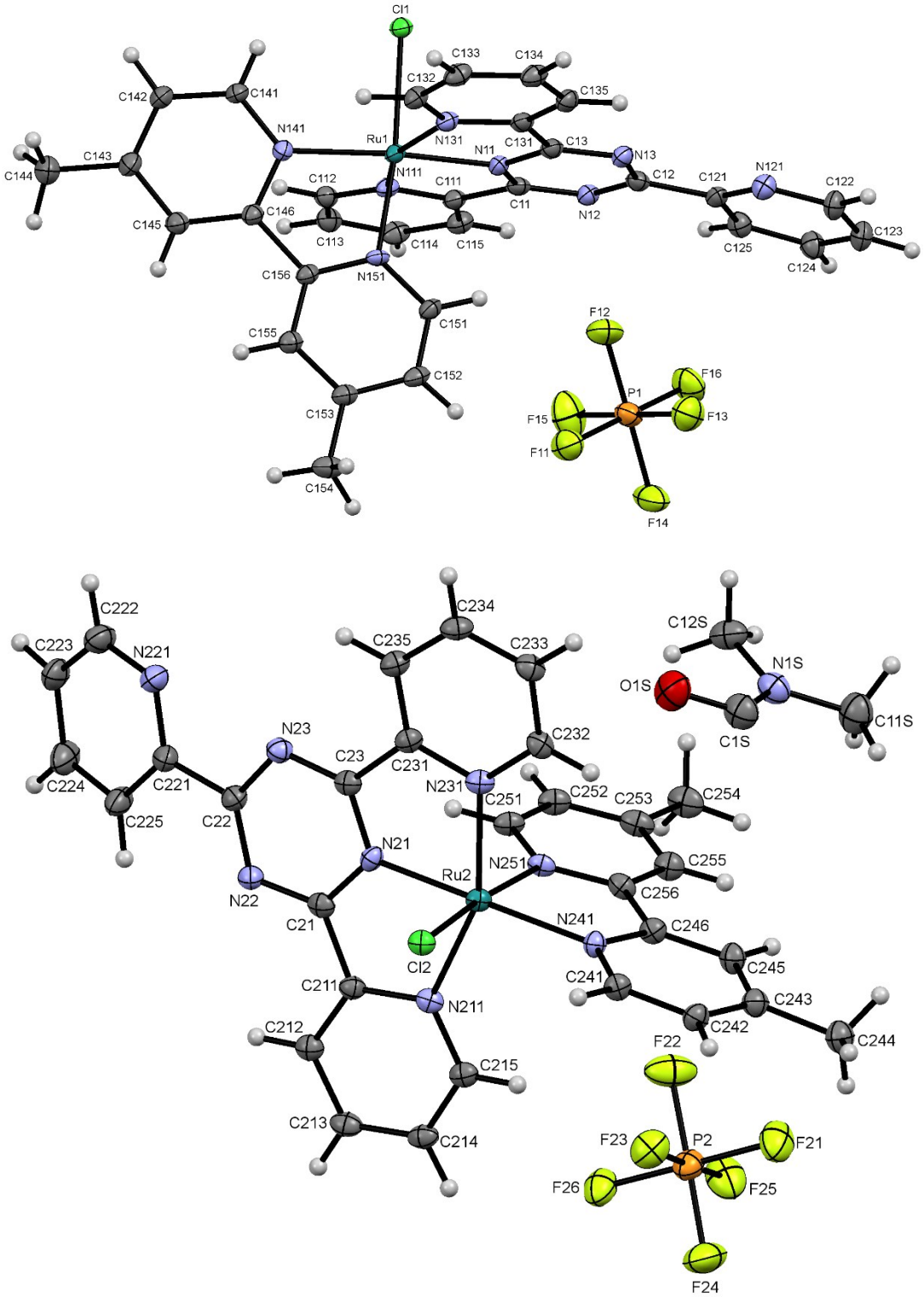


Fig. S1 Views of both cations including the anions and the ordered DMF solvate.

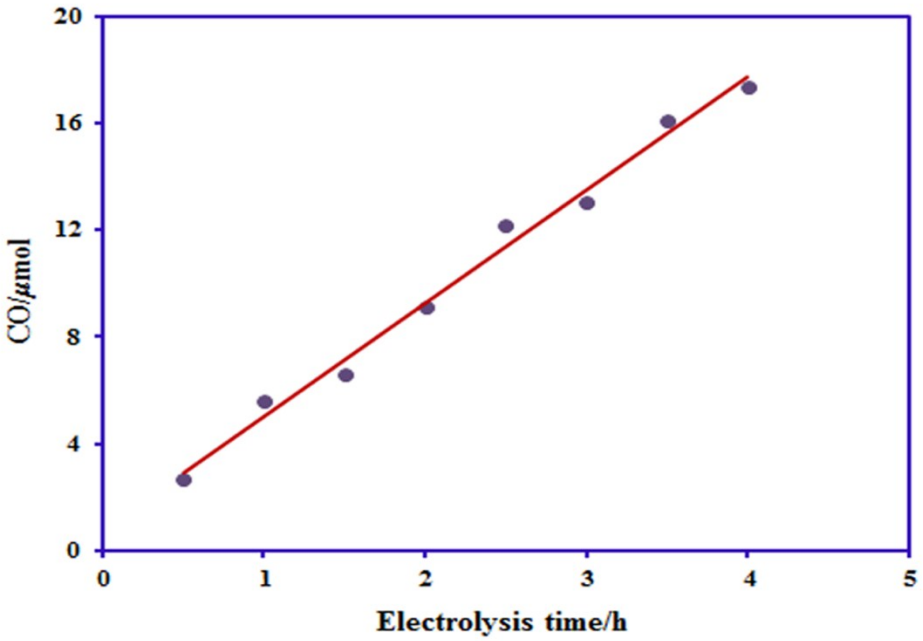


Fig. S2 Formation of CO during the electrolysis process in the presence of the Ru(II) electrocatalyst.

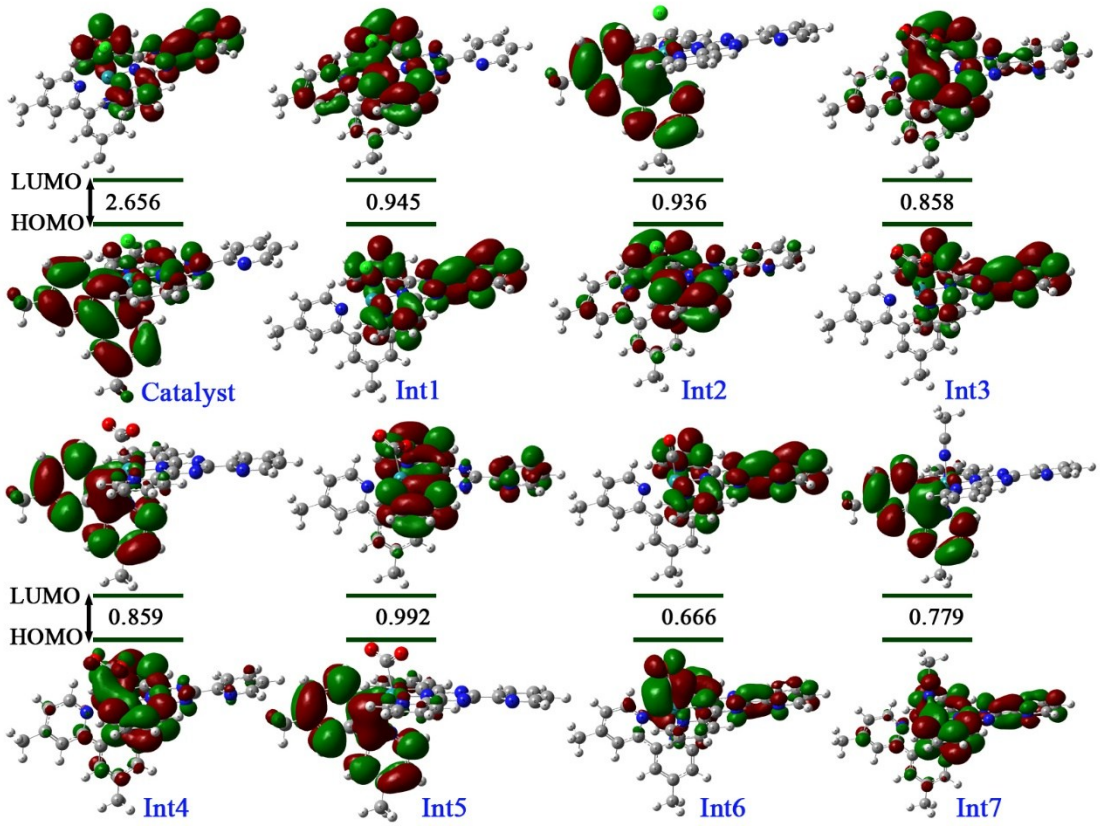
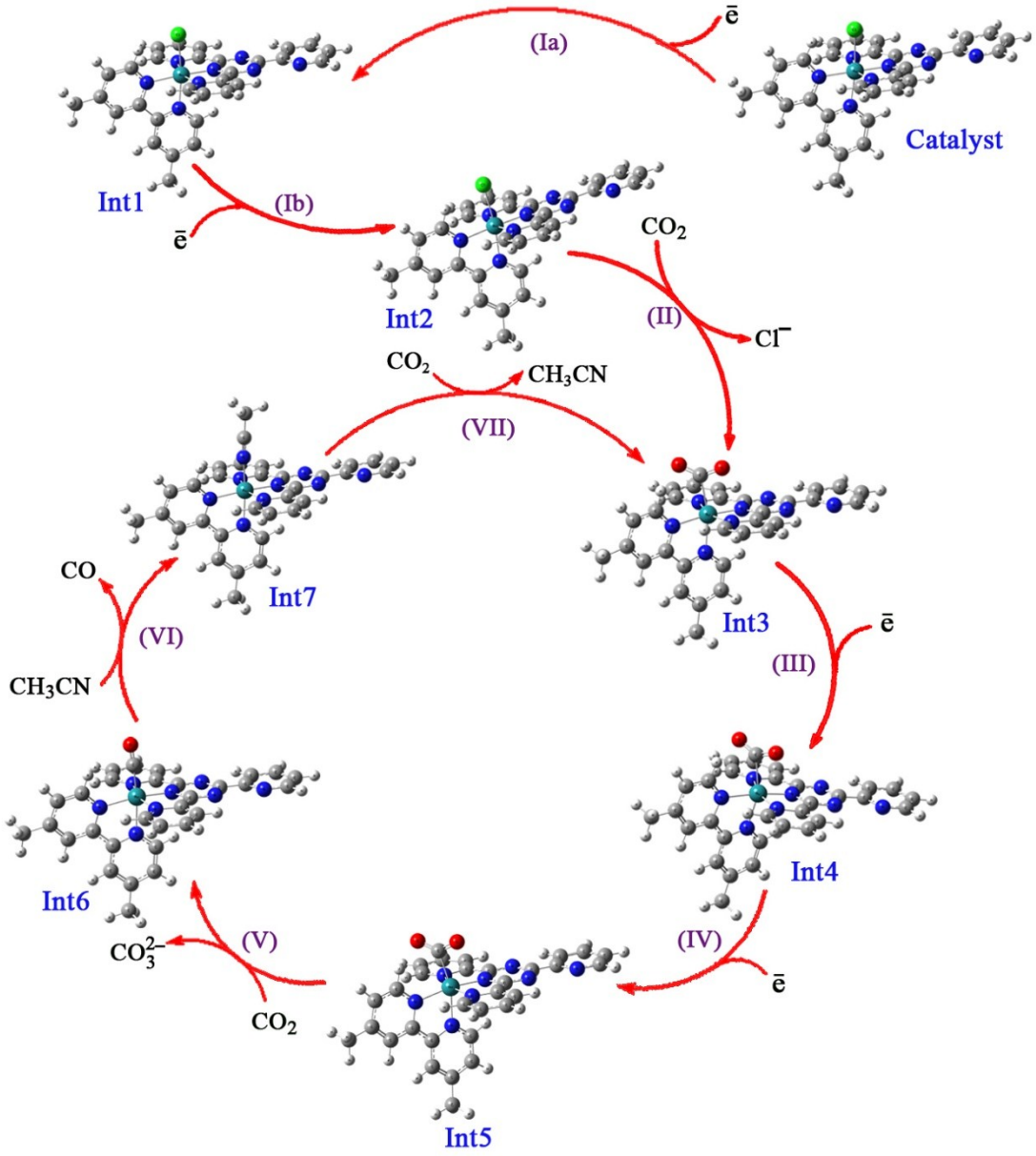


Fig. S3 The distribution and energy (eV) of the FMOs of the species involved in the electrocatalytic cycle in the gas phase.

Table S1. Bond lengths [Å] and angles [°] for [Ru(dmbpy)(tptz)(Cl)](PF_6)·0.5DMF

Ru(1)-N(11)	1.946(4)	C(125)-H(125)	0.9500
Ru(1)-N(151)	2.047(3)	C(131)-N(131)	1.363(6)
Ru(1)-N(111)	2.077(4)	C(131)-C(135)	1.391(7)
Ru(1)-N(141)	2.083(4)	N(131)-C(132)	1.354(6)
Ru(1)-N(131)	2.086(4)	C(132)-C(133)	1.387(7)
Ru(1)-Cl(1)	2.4014(10)	C(132)-H(132)	0.9500
N(11)-C(11)	1.338(6)	C(133)-C(134)	1.382(8)
N(11)-C(13)	1.340(6)	C(133)-H(133)	0.9500
C(11)-N(12)	1.324(6)	C(134)-C(135)	1.388(8)
C(11)-C(111)	1.471(6)	C(134)-H(134)	0.9500
N(12)-C(12)	1.348(6)	C(135)-H(135)	0.9500
C(12)-N(13)	1.345(7)	N(141)-C(141)	1.343(6)
C(12)-C(121)	1.485(6)	N(141)-C(146)	1.361(6)
N(13)-C(13)	1.323(6)	C(141)-C(142)	1.385(7)
C(13)-C(131)	1.464(7)	C(141)-H(141)	0.9500
N(111)-C(112)	1.343(6)	C(142)-C(143)	1.402(7)
N(111)-C(111)	1.378(6)	C(142)-H(142)	0.9500
C(111)-C(115)	1.385(7)	C(143)-C(145)	1.386(7)
C(112)-C(113)	1.379(7)	C(143)-C(144)	1.519(7)
C(112)-H(112)	0.9500	C(144)-H(14A)	0.9800
C(113)-C(114)	1.371(8)	C(144)-H(14B)	0.9800
C(113)-H(113)	0.9500	C(144)-H(14C)	0.9800
C(114)-C(115)	1.393(7)	C(145)-C(146)	1.391(7)
C(114)-H(114)	0.9500	C(145)-H(145)	0.9500
C(115)-H(115)	0.9500	C(146)-C(156)	1.485(6)
C(121)-N(121)	1.344(7)	N(151)-C(151)	1.346(6)
C(121)-C(125)	1.399(7)	N(151)-C(156)	1.359(6)
N(121)-C(122)	1.328(7)	C(151)-C(152)	1.371(7)
C(122)-C(123)	1.391(8)	C(151)-H(151)	0.9500
C(122)-H(122)	0.9500	C(152)-C(153)	1.409(7)
C(123)-C(124)	1.391(8)	C(152)-H(152)	0.9500
C(123)-H(123)	0.9500	C(153)-C(155)	1.392(7)
C(124)-C(125)	1.379(7)	C(153)-C(154)	1.490(7)
C(124)-H(124)	0.9500	C(154)-H(15A)	0.9800



Scheme S1 The optimized structures of the species involved in the electrocatalytic cycle in the gas phase.