Supplementary material

This table presents the c_{ijklmn} coefficients of the 6D-potential energy expansion of the average component (i.e. (^{2}A' + ^{2}A") /2) of the $OMgOO^+(X^2\Pi)$ state computed at the RCCSD(T)-F12/cc-pVTZ-F12 level of theory

Table S1: c_{ijklmn} coefficients for the average component (^{2}A' + ^{2}A") /2

i	j	k	l	m	n	c_{ijklmn}
0	0	0	0	0	0	-4.2464503041e+02
1	0	0	0	0	0	8.4612209035e-07
2	0	0	0	0	0	3.4740489605e-01
3	0	0	0	0	0	-5.0827755954e-01
4	0	0	0	0	0	3.5106263629e-01
0	1	0	0	0	0	-2.7825325100e-09
0	2	0	0	0	0	9.9661875115e-02
0	3	0	0	0	0	-9.1174529224e-02
0	4	0	0	0	0	4.2633814606e-02
0	0	1	0	0	0	1.7077158021e-08
0	0	2	0	0	0	2.0726118828e-02
0	0	3	0	0	0	-2.1778763819e-02
0	0	4	0	0	0	1.3499110185e-02
0	0	5	0	0	0	-5.2288051893e-03
0	0	6	0	0	0	9.0423406062e-04
0	0	0	2	0	0	-1.5197857392e-02
0	0	0	4	0	0	9.9134172705e-03
0	0	0	6	0	0	-1.7165197374e-03
0	0	0	8	0	0	-2.6121625726e-04
0	0	0	10	0	0	7.5215018842e-05
0	0	0	12	0	0	1.4809303318e-06
0	0	0	0	2	0	2.1361986642e-03
0	0	0	2	2	0	-1.5640102302e-03
0	0	0	4	2	0	6.8504079331e-04
0	0	0	10	2	0	-4.4839756217e-06
0	0	0	0	4	0	1.5380935246e-03
0	0	0	4	4	0	-2.2288161450e-04
0	0	0	8	4	0	1.4297120500e-05
0	0	0	0	6	0	-7.6505784968e-04

0 0 0 2 6 0 -3.1249005193e-05

0 0 0 4 6 0 1.2644096795e-04

0 0 0 0 8 0 2.1236512621e-04

0 0 0 1 1 1 2.4025898830e-03

0 0 0 3 1 1 -3.6369481185e-03

0 0 0 5 1 1 5.3811754520e-04

0 0 0 7 1 1 5.1139150885e-04

0 0 0 9 1 1 -1.4766939436e-04

0 0 0 11 1 1 1.0104281976e-05

0 0 0 1 3 1 1.7760049345e-03

0 0 0 3 3 1 -1.4764720347e-03

0 0 0 5 3 1 3.6871801976e-04

0 0 0 7 3 1 -3.8191942494e-05

0 0 0 1 5 1 -6.8486369392e-04

0 0 0 5 5 1 1.2529554103e-04

0 0 0 1 7 1 1.7032005494e-04

1 0 0 2 0 0 -9.7726392158e-03

2 0 0 2 0 0 4.4573034775e-03

0 0 1 2 0 0 -1.2190049948e-02

0 0 2 2 0 0 1.2521257520e-02

0 0 3 2 0 0 -4.7922144366e-03

0 0 4 2 0 0 1.7317514276e-03

0 0 1 4 0 0 5.6321735506e-03

0 0 2 4 0 0 -3.6938621761e-03

0 0 3 4 0 0 1.1797094199e-03

0 0 4 4 0 0 -6.0349771337e-04

0 0 1 6 0 0 -9.4450136065e-04

0 0 2 6 0 0 -5.0338962316e-04

0 0 1 8 0 0 8.7770263967e-05

0 0 2 8 0 0 2.7120945498e-04

0 0 1 12 0 0 -1.0392397552e-05

0 0 2 12 0 0 2.9588243828e-06

0 0 1 0 2 0 -2.1448398593e-03

0 0 2 0 2 0 -2.3050960073e-03

0 0 3 0 2 0 5.8960645750e-04

0 0 4 0 2 0 -3.4029709264e-04

0 0 1 2 2 0 3.6926495308e-03

0 0 2 2 2 0 -1.1801404099e-04

0 0 1 4 2 0 -1.1111262893e-03

0 0 2 4 2 0 1.1077064789e-04

0 0 1 0 4 0 1.1206133186e-03

0 0 2 0 4 0 1.4282111808e-03

0 0 1 2 4 0 -8.1791592572e-04

0 0 2 2 4 0 1.0585376073e-05

0 0 1 0 6 0 -4.9166671701e-04

0 0 2 0 6 0 -1.6892762681e-04

0 0 1 1 1 1 -1.0722344091e-03

0 0 2 1 1 1 -3.9536767471e-03

0 0 1 3 1 1 1.7458737048e-03

0 0 2 3 1 1 4.0620883479e-03

0 0 1 5 1 1 -5.7450568341e-04

0 0 2 5 1 1 -1.6693936599e-03

0 0 1 7 1 1 4.1931857609e-05

0 0 2 7 1 1 2.5943589005e-04

0 0 1 1 3 1 1.5885567532e-03

0 0 2 1 3 1 1.0934239094e-03

0 0 1 3 3 1 -9.4992483080e-04

0 0 2 3 3 1 -1.8027679782e-05

0 0 1 1 5 1 -3.6976236913e-04

0 0 2 1 5 1 -1.5427177943e-04

This table presents the c_{ijklmn} coefficients of the 6D-potential energy expansion of the difference (^{2}A' - ^{2}A")/2 component of the OMgOO$^+$($X^2\Pi$) state computed at the RCCSD(T)-F12/cc-pVTZ-F12 level of theory

Table S2: c_{ijklmn} coefficients for the difference (^{2}A' - ^{2}A")/2 component for *cis* configuration and (^{2}A" - ^{2}A')/2 for *trans* configuration

i	j	k	l	m	n	c_{ijklmn}
0	0	0	3	1	0	3.2762358861e-04
0	0	0	5	1	0	-7.1001699502e-05
0	0	0	4	2	0	-1.1439787463e-03
0	0	0	6	2	0	1.4541938769e-04
0	0	0	1	3	0	-9.1295686876e-04
0	0	0	3	3	0	2.6349629589e-03
0	0	0	4	4	0	-8.4583686008e-04
0	0	0	1	0	1	1.0704520792e-04
0	0	0	2	0	1	-2.7805146128e-05
0	0	0	3	1	1	3.8295485861e-04
0	0	0	0	2	1	-7.1768363240e-04
0	0	0	2	2	1	2.4549807736e-04
0	0	0	4	2	1	-1.2862201239e-03
0	0	0	1	3	1	-4.6989898930e-04
0	0	0	3	3	1	1.8420258344e-03
0	0	0	5	3	1	5.4084315370e-04
0	0	0	0	4	1	-4.8669242017e-04
0	0	0	2	4	1	6.2650535548e-04
0	0	0	4	4	1	-1.2396789963e-03
0	0	0	0	6	1	2.0238855097e-04
0	0	0	0	8	1	-1.0817267675e-04
0	0	1	2	2	0	-1.8961186643e-03
0	0	2	2	2	0	4.0916938397e-04
0	0	1	3	3	0	1.4354200897e-03
0	0	2	3	3	0	-4.1368015355e-04
0	0	1	1	1	1	1.7693819823e-03
0	0	1	0	2	1	6.8779785919e-04
0	0	2	0	2	1	-6.2876130618e-04
0	0	1	2	2	1	-3.5272414240e-03
0	0	2	2	2	1	9.6017541720e-04
0	0	1	1	3	1	-9.5006983718e-04

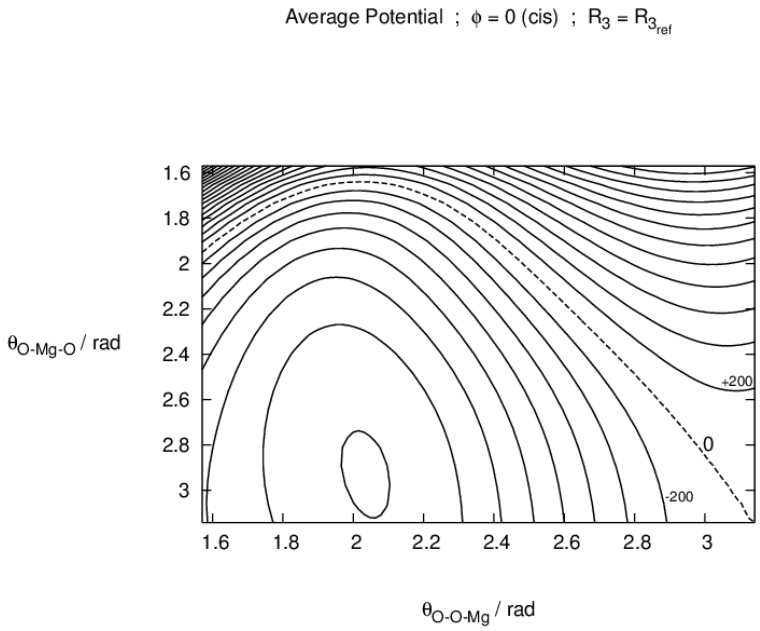
0 0 2 1 3 1 -1.4011285561e-04

0 0 1 3 3 1 2.0018910525e-03

0 0 2 3 3 1 -5.1915385586e-04

0 0 1 0 6 1 2.8255827168e-04

Figure S1: 2D cuts of the RCCSD(T)-F12/cc-pVTZ-F12 6D-PESs of the $OMgOO^{+}(^{2}\Pi)$ average potential along the in-plane angles (θ_1,θ_2) for *cis* (Φ = 0°) and *trans* (Φ = 180°) configurations. The step between the contours is 200 cm^{-1}. The zero energy corresponds to the minimum energy for linear configuration (i.e. for R_1^{Ref} = 2.293, R_2^{Ref} = 3.451 and R_3^{Ref} = 3.977 , in bohr; and θ_1=θ_2 = 180°).



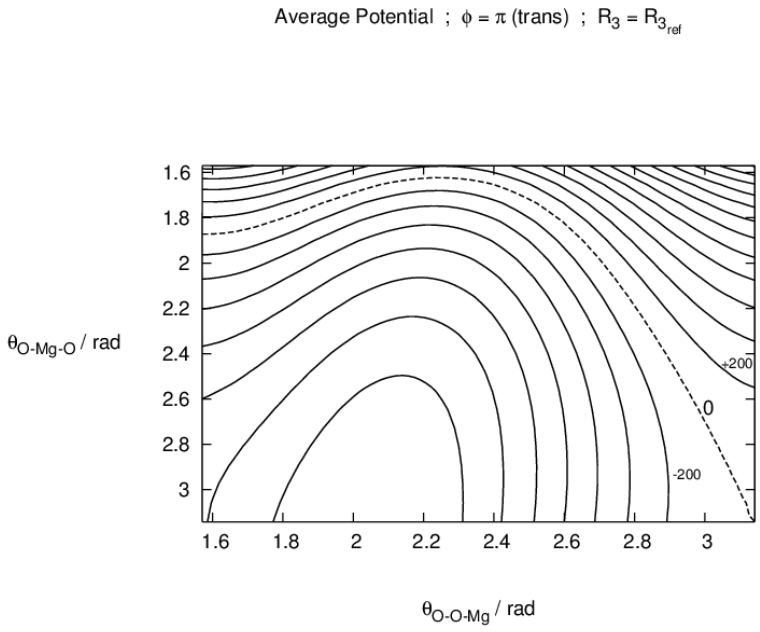


Figure S2: 2D cuts of the RCCSD(T)-F126D-potential energy expansion 6D-PESs of the $OMgOO^+(^2\Pi)$ average potential along the in-plane angles (θ_1,θ_2) for cis (Φ = 0°) and trans (Φ = 180°) configurations. The step between the contours is 200 cm^{-1}. The zero energy corresponds to the minimum energy for linear configuration (i.e. for R_1^{Ref} = 2.293, R_2^{Ref} = 3.451 and R_3^{Ref} = 3.977 + 0.5, in bohr; and θ_1=θ_2 = 180°).