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Supporting Information

Ab initio investigation of the ground and excited states of $MoO^{+,2+,-}$ and their catalytic strength on water activation

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Figure S1. MRCI PECs of MoO^{2+} with respect to the Mo-O distance in the range 1.0 to 30.0 Å. The ^3X states can be one of ^3P, ^3H, ^3F, or ^3G.

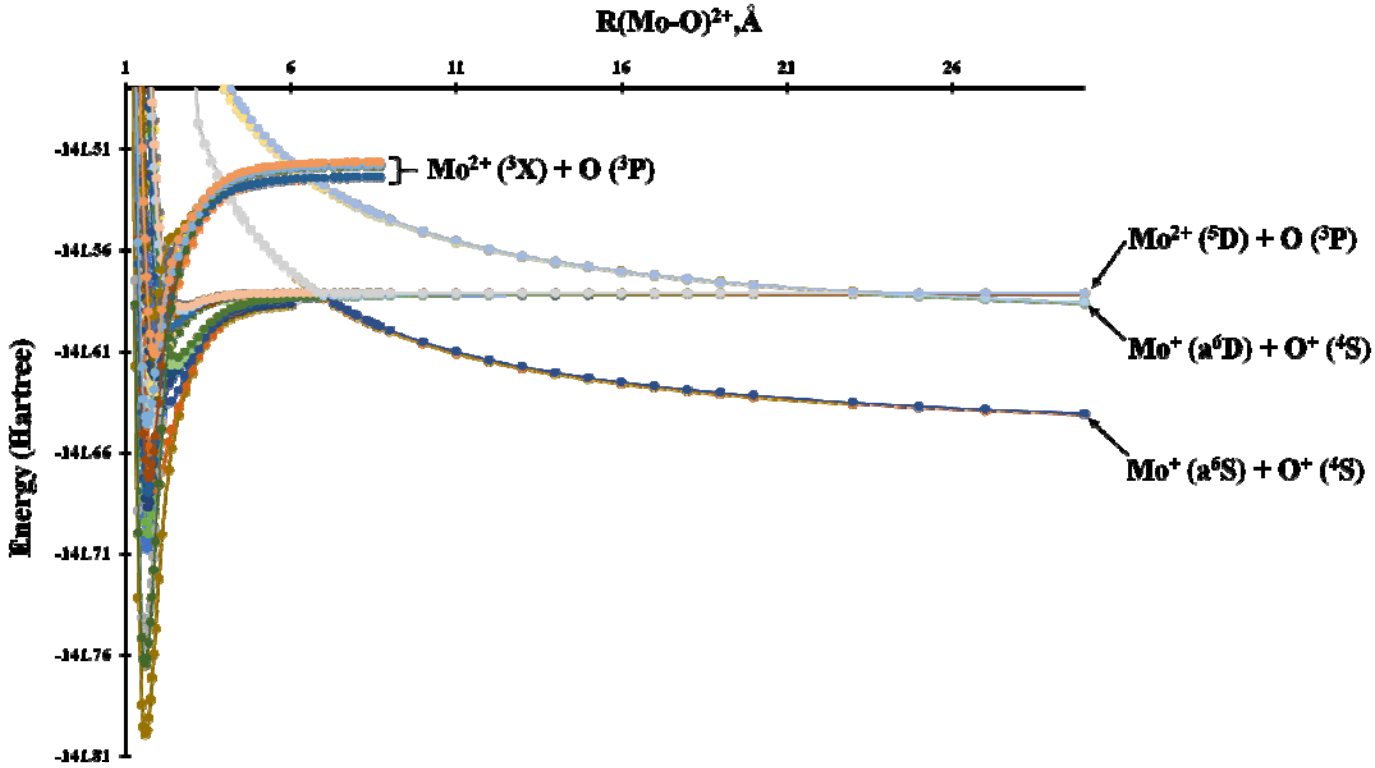

Table S1. Optimal geometries for $MoO^{+,2+,-}$ (MoO distance in Å) water-$MoO^{+,2+,-}$ interacting complex (reactants), transition states (TS), and products ($HOMoOH^{+,2+,-}$) at the MRCI/triple-ζ (see text) level of theory (Cartesian coordinates in Å) for the lowest electronic states.

Species	MoO	Reactants	TS	Product
MoO^{+}	1.613	Mo 0.3081520000 0.3259430000 0.1232980000	Mo 0.4394990000 -0.1646950000 -0.0058630000	Mo -0.6109610000 0.0232790000 0.0128640000
$X^4\Sigma^-$		O 1.1500430000 1.6901790000 -0.1467370000	O -0.2943990000 1.4081270000 0.0194460000	O -0.2037220000 1.7694110000 -0.0920590000
		O -1.7618600000 -0.4025070000 0.1622060000	O -1.5614110000 -0.4528370000 -0.0847430000	O -1.5309610000 -1.5025520000 0.2390640000
(1^4A)		H -2.5324340000 0.1287890000 -0.0455010000	H -1.3226490000 0.7993570000 0.0211120000	H -0.2315160000 2.7251200000 -0.0914410000
		H -2.0768820000 -1.2810740000 0.3827100000	H -2.1422990000 -0.9096680000 0.5176320000	H -2.2091340000 -2.1553380000 0.4066830000
MoO^{+}	1.597	Mo 0.2741890000 0.3643750000 -0.3873540000	Mo 0.4377060000 -0.1647420000 -0.0104090000	Mo -0.9548470000 0.1583050000 0.0812780000
$a^2\Delta$		O 1.0779680000 1.5519050000 0.3268080000	O -0.3088910000 1.3840030000 0.0430720000	O -0.3117860000 1.8228770000 -0.1236440000
		O -1.7501100000 -0.4125840000 0.0385740000	O -1.5552300000 -0.4633960000 -0.0996480000	O -1.6060920000 -1.5027330000 0.2890060000
(1^2A)		H -2.5713680000 -0.0197510000 -0.2561000000	H -1.3271430000 0.8138600000 0.0007090000	H 0.0268220000 2.7089950000 -0.2286400000
		H -1.9717630000 -1.0307060000 0.7345110000	H -2.1277010000 -0.8894430000 0.5338600000	H -1.9553890000 -2.3836320000 0.4025590000
MoO^{+}	1.597	Mo 0.3090880000 0.3924500000 0.0492000000	Mo 0.4196090000 -0.1688780000 -0.0023140000	Mo -0.9546960000 0.1582430000 0.0812480000
$a^2\Delta$		O 1.2448010000 1.6925950000 -0.0120130000	O -0.3149230000 1.3830110000 0.0596750000	O -0.3118270000 1.8228890000 -0.1236760000
		O -1.7992330000 -0.4345050000 0.1164730000	O -1.5781490000 -0.4860260000 -0.1424130000	O -1.6061300000 -1.5027200000 0.2889950000
(2^2A)		H -2.5646110000 0.0524000000 -0.1899280000	H -1.3144520000 0.8261860000 -0.0084040000	H 0.0267860000 2.7090100000 -0.2285960000
		H -2.1311290000 -1.2497010000 0.4927080000	H -2.0933420000 -0.8740090000 0.5610400000	H -1.9554240000 -2.3836100000 0.4025880000
MoO^{+}	1.656	Mo 0.3081520000 0.3259430000 0.1232980000	Mo 0.4394990000 -0.1646950000 -0.0058630000	Mo -0.6109610000 0.0232790000 0.0128640000
$A^4\Pi$		O 1.1500430000 1.6901790000 -0.1467370000	O -0.2943990000 1.4081270000 0.0194460000	O -0.2037220000 1.7694110000 -0.0920590000
		O -1.7618600000 -0.4025070000 0.1622060000	O -1.5614110000 -0.4528370000 -0.0847430000	O -1.5309610000 -1.5025520000 0.2390640000
(1^4A)		H -2.5324340000 0.1287890000 -0.0455010000	H -1.3226490000 0.7993570000 0.0211120000	H -0.2315160000 2.7251200000 -0.0914410000
		H -2.0768820000 -1.2810740000 0.3827100000	H -2.1422990000 -0.9096680000 0.5176320000	H -2.2091340000 -2.1553380000 0.4066830000
MoO^{+}	1.656	Mo 1.6793100000 0.9537550000 0.2014780000	Mo 0.5346230000 -0.1679250000 0.0106550000	Mo 0.4655260000 -0.3490150000 -0.1436930000
$A^4\Pi$		O 0.1067280000 0.4498760000 -0.2185150000	O -0.3378990000 1.3915380000 0.1098030000	O -0.5241160000 1.3683820000 -0.3629300000
		O -2.5350320000 -0.3519090000 -0.0932080000	O -1.7141620000 -0.4329280000 -0.2200670000	O 1.4438150000 -2.0690490000 0.1486720000
(2^4A)		H -1.6232700000 -0.0662730000 -0.2509790000	H -1.3378090000 0.6609040000 -0.0452000000	H -0.7829470000 1.8183410000 0.4328520000
		H -2.5726470000 -0.4207300000 0.8522580000	H -2.0260120000 -0.7713060000 0.6123930000	H 0.9098730000 -2.8471610000 0.2578130000
MoO^{2+}	1.568	Mo 0.3273550000 0.1795210000 0.0345080000	Mo 0.3926340000 -0.1997000000 0.0064530000	Mo -0.5684050000 -0.0088340000 0.0298100000
$X^3\Sigma^-$		O 0.9658370000 1.6052930000 -0.1134630000	O -0.2647820000 1.3471240000 -0.0338230000	O -0.2693680000 1.7017890000 -0.1455930000
		O -1.7308460000 -0.3656170000 0.1492780000	O -1.5234370000 -0.3879510000 0.0393010000	O -1.4610300000 -1.4858100000 0.2904240000
(1^3A)		H -2.4707260000 0.2320420000 -0.0352760000	H -1.3644030000 0.9579790000 0.0169110000	H -0.3184200000 2.6755860000 -0.2073210000
		H -2.1272360000 -1.2093410000 0.4124200000	H -2.1212700000 -1.0371700000 0.4387410000	H -2.1322780000 -2.1761370000 0.4559250000
MoO^{2+}	1.565	Mo 0.3281160000 0.1581510000 -0.3155230000	Mo 0.3086990000 -0.1485390000 -0.0068560000	Mo -0.5030710000 -0.0048600000 0.0224790000
$\alpha^1\Gamma$		O 0.6604460000 1.5045170000 0.4186710000	O -0.2342210000 1.4279330000 0.0706410000	O -0.2336470000 1.7069550000 -0.1502190000
		O -1.6406570000 -0.3638600000 0.0216390000	O -1.5277740000 -0.5678630000 -0.1246520000	O -1.4879120000 -1.4165030000 0.2871940000
(1^1A)		H -2.4041880000 -0.0424310000 -0.4655990000	H -1.3084360000 0.8794600000 -0.0355490000	H -0.3119810000 2.6794680000 -0.2104110000
		H -1.9806920000 -0.8394920000 0.7848170000	H -2.1195260000 -0.9107080000 0.5640000000	H -2.2119920000 -2.0520740000 0.4524200000
MoO^{2+}	1.565	Mo 0.3392870000 0.1437440000 -0.0458690000	Mo 0.3906310000 -0.1969620000 0.0135680000	Mo -0.5001040000 -0.0356650000 0.0201150000
$\alpha^1\Gamma$		O 0.9728660000 1.5663290000 -0.2408590000	O -0.2608120000 1.3364150000 -0.0601460000	O -0.2707750000 1.6827650000 -0.1446530000
		O -1.6995800000 -0.3894890000 0.2361970000	O -1.5306610000 -0.3886510000 0.0732400000	O -1.4495120000 -1.4708460000 0.2877730000
(2^1A)		H -2.4347620000 0.2413140000 0.2649810000	H -1.3532470000 0.9997600000 0.0240950000	H -0.3714960000 2.6537480000 -0.1961960000
		H -2.0925040000 -1.2658890000 0.3647920000	H -2.1271690000 -1.0702790000 0.4168270000	H -2.1576130000 -2.1234060000 0.4562060000

MoO^-	1.700	Mo 1.7268250000 0.9725020000 0.0127210000	Mo 0.5567710000 -0.1762400000 0.0152230000	Mo 0.4665680000 -0.3493840000 -0.1235290000
$X\ ^4\Pi$		O 0.1060700000 0.4444950000 0.0437250000	O -0.3497050000 1.3937810000 0.0756320000	O -0.2610930000 1.4834110000 -0.2417700000
		O -2.5254740000 -0.3451810000 -0.1464110000	O -1.7096660000 -0.4363090000 -0.1976700000	O 1.3173990000 -2.1321930000 -0.1413160000
(1^4A)		H -1.6019300000 -0.0585790000 -0.2072990000	H -1.3191730000 0.7128970000 -0.0198790000	H -0.9730620000 1.6769180000 0.3581510000
		H -2.6504020000 -0.4485180000 0.7883000000	H -2.0594850000 -0.8138460000 0.5942790000	H 0.9623390000 -2.7572540000 0.4811780000
MoO^-	1.700	Mo 1.6793100000 0.9537550000 0.2014780000	Mo 0.5346230000 -0.1679250000 0.0106550000	Mo 0.4655260000 -0.3490150000 -0.1436930000
$X\ ^4\Pi$		O 0.1067280000 0.4498760000 -0.2185150000	O -0.3378990000 1.3915380000 0.1098030000	O -0.5241160000 1.3683820000 -0.3629300000
		O -2.5350320000 -0.3519090000 -0.0932080000	O -1.7141620000 -0.4329280000 -0.2200670000	O 1.4438150000 -2.0690490000 0.1486720000
(2^4A)		H -1.6232700000 -0.0662730000 -0.2509790000	H -1.3378090000 0.6609040000 -0.0452000000	H -0.7829470000 1.8183410000 0.4328520000
		H -2.5726470000 -0.4207300000 0.8522580000	H -2.0260120000 -0.7713060000 0.6123930000	H 0.9098730000 -2.8471610000 0.2578130000
MoO^-	1.741	Mo 1.7355940000 0.9770170000 -0.0025390000	Mo 0.7321230000 -0.1025130000 -0.0212440000	Mo 0.3681950000 -0.3891720000 -0.0096800000
$1^6\Sigma^+$		O 0.0578670000 0.4283910000 0.0481860000	O -0.3479900000 1.3906220000 0.1190330000	O -0.1754040000 1.6415530000 -0.0130220000
		O -2.5055450000 -0.3377280000 -0.1535840000	O -1.7970430000 -0.4464940000 -0.2137910000	O 1.1413660000 -2.3271010000 -0.2665750000
(1^6A)		H -1.5695600000 -0.0510690000 -0.1758310000	H -1.3256110000 0.5784080000 -0.0373870000	H -1.0934200000 1.8470310000 0.1084680000
		H -2.6632650000 -0.4518920000 0.7748040000	H -2.1427370000 -0.7397400000 0.6209730000	H 1.2714140000 -2.8508130000 0.5135230000
MoO^-	1.646	Mo 1.6191550000 0.7094130000 0.2756280000	Mo 0.5151890000 -0.1661450000 0.0044900000	Mo 0.6771930000 -0.2415980000 -0.3252510000
$1^2\Delta$		O 0.0703510000 0.7885670000 -0.2889600000	O -0.3412960000 1.4020820000 0.1086610000	O -0.2719000000 1.3351750000 0.0405480000
		O -2.5568740000 -0.2631620000 -0.0015540000	O -1.6847970000 -0.4486450000 -0.2121150000	O 1.4382080000 -1.9802030000 -0.7008310000
(1^2A)		H -1.7225090000 0.1730780000 -0.1996020000	H -1.3362710000 0.6619030000 -0.0453270000	H -1.0880320000 1.7546820000 0.1983880000
		H -2.3187660000 -0.8631080000 0.6944460000	H -2.0340830000 -0.7689120000 0.6118740000	H 1.0105560000 -2.8208090000 -0.8076610000
MoO^-	1.646	Mo 1.6219660000 0.7126290000 0.2735090000	Mo 0.5024020000 -0.1779250000 0.0143440000	Mo 0.6788570000 -0.2407820000 -0.3252060000
$1^2\Delta$		O 0.0714640000 0.7868370000 -0.2872780000	O -0.3222660000 1.4161780000 0.1085010000	O -0.2725480000 1.3342910000 0.0405150000
		O -2.5574180000 -0.2622910000 -0.0022620000	O -1.6863400000 -0.4318030000 -0.2166540000	O 1.4376960000 -1.9802020000 -0.7008970000
(2^2A)		H -1.7211870000 0.1718220000 -0.1975260000	H -1.3675300000 0.6456240000 -0.0504820000	H -1.0881440000 1.7547760000 0.1983490000
		H -2.3234680000 -0.8642080000 0.6935150000	H -2.0075240000 -0.7717910000 0.6118750000	H 1.0101620000 -2.8208360000 -0.8075660000