Performance of density functional theory for second row (4*d*) transition metal thermochemistry

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Table 1S. Atomic enthalpies of formation at 0 K.[1] Units are in kcal mol^{-1}.

Atom	ΔH_f(0K)
Ag	67.982
Br	28.18
C	170.112
Cd	26.73
Cl	28.59
F	18.47
H	51.63
Mo	156.517
Nb	171.958
O	58.99
Pd	88.8
Rh	132.7
Ru	156.6
Y	100.887
Zr	143.093

Table 2S. The enthalpies of formation (ΔH_f's) for the TM-4*d* set as determined by the Generalized Gradient Approximation (GGA) functionals. See Reference 2 for more details about the experimental data and uncertainties. Units are in kcal mol^{-1}.

Molecule	BLYP	BP86	PBEPBE	TPSSKCIS	M06L	Experiment
AgH	64.17	61.48	64.82	65.28	65.49	*66.30*
Cd_2	53.38	52.72	52.16	52.61	51.17	*51.40*
CdBr	22.87	17.39	16.03	15.93	20.21	*15.89*
$CdBr_2$	-24.40	-35.36	-38.05	-36.42	-32.45	*-33.45±1.1*
CdCl	17.79	12.19	10.54	10.28	9.71	*6.55*
$CdCl_2$	-36.32	-47.39	-50.56	-49.04	-55.89	*-46.50±1.1*
CdH	73.77	68.89	71.80	69.92	74.41	*62.30*
$MoCO_5$	-192.29	-239.57	-252.02	-193.83	-184.66	*-157.50±5.0*
$MoCO_6$	-255.68	-313.06	-328.40	-259.61	-246.83	*-218.95±1.1*
MoF	54.91	56.08	56.48	57.74	61.73	*67.60±3.0*
MoF_2	-52.70	-51.25	-50.30	-47.10	-39.59	*-38.90±4.0*
MoF_6	-432.94	-441.92	-443.87	-426.46	-406.00	*-372.30±2.2*
MoO_2	-31.51	-34.00	-32.31	-20.49	-10.16	*-1.98±3.0*
MoO_2Cl_2	-175.18	-187.37	-188.13	-171.23	-172.63	*-151.60±3.5*
MoO_3	-112.67	-118.12	-117.54	-99.42	-86.16	*-86.70±5.0*
$MoOCl_4$	-151.79	-170.23	-173.05	-158.62	-171.56	*-135.90±1.4*
NbO	41.00	39.02	39.77	46.63	48.75	*47.50±5.0*
NbO_2	-64.53	-68.43	-67.93	-54.97	-50.97	*-47.80±5.0*
RhC	154.84	147.07	145.07	156.84	158.90	*164.10±2.3*
$RhCl_2$	30.22	20.97	17.77	27.07	17.17	*30.00±3.0*
RhO	76.51	72.36	70.68	82.15	86.55	*95.00±10.0*
RuO_4	-138.85	-160.14	-163.78	-129.17	-93.13	*-46.03±1.0*
YO	-15.15	-21.60	-21.59	-14.47	-3.75	*-11.00±2.5*
ZrBr	73.41	69.05	65.01	66.88	72.50	*71.90±0.5*
$ZrBr_4$	-155.01	-176.00	-181.18	-173.45	-165.74	*-166.00±2.0*
ZrCl	62.17	57.11	55.46	58.00	55.02	*67.59±5.7*
$ZrCl_2$	-29.63	-41.44	-44.59	-42.28	-43.76	*-34.87±3.6*
$ZrCl_4$	-201.86	-222.00	-228.05	-220.71	-235.34	*-208.03±0.6*
ZrO	13.42	7.75	6.67	17.32	25.72	*21.80*
ZrO_2	-85.79	-98.18	-101.02	-86.68	-73.33	*-68.40±11.0*

Table 3S. The enthalpies of formation (ΔH_f's) for the TM-4*d* set as determined by the hybrid GGA (HGGA) functionals. See Reference 2 for more details about the experimental data and uncertainties. Units are in kcal mol^{-1}.

Molecule	B3P86	B3LYP	B971	X3LYP	PBE1PBE	mPW1LYP	B1LYP	M06	BMK	M062X	Experiment
AgH	63.83	66.16	65.72	66.30	68.66	67.40	67.89	67.26	66.99	72.57	*66.30*
Cd_2	52.47	53.14	52.07	52.96	52.29	52.92	53.31	51.06	52.41	52.15	*51.40*
CdBr	15.32	20.68	18.71	20.20	14.39	20.69	21.39	25.32	22.06	17.41	*15.89*
$CdBr_2$	-39.11	-28.72	-36.47	-29.80	-39.99	-28.54	-26.80	-25.47	-33.39	-34.75	*-33.45±1.1*
CdCl	10.11	15.65	13.02	15.21	9.15	15.81	16.51	16.44	13.72	9.45	*6.55*
$CdCl_2$	-50.95	-40.31	-49.68	-41.31	-51.68	-39.78	-38.03	-45.89	-52.16	-51.68	*-46.50±1.1*
CdH	66.97	71.50	74.91	71.48	69.80	72.04	72.12	78.64	76.06	73.21	*62.30*
$MoCO_5$	-187.07	-139.26	-183.02	-140.23	-149.89	-116.21	-100.30	-174.45	-184.14	-142.93	*-157.50±5.0*
$MoCO_6$	-254.26	-196.51	-246.14	-198.08	-211.76	-170.12	-151.10	-238.41	-248.00	-201.43	*-218.95±1.1*
MoF	61.75	61.34	58.74	61.08	66.65	62.38	64.07	63.77	50.22	58.83	*67.60±3.0*
MoF_2	-39.83	-40.16	-43.93	-40.68	-29.88	-37.91	-34.57	-37.10	-58.29	-44.10	*-38.90±4.0*
MoF_6	-394.38	-383.82	-399.34	-383.99	-365.01	-370.64	-360.67	-392.14	-397.87	-361.96	*-372.30±2.2*
MoO_2	-3.43	-0.08	-12.12	1.06	14.07	8.49	12.47	-3.04	-16.15	8.12	*-1.98±3.0*
MoO_2Cl_2	-151.98	-139.79	-163.33	-139.26	-131.47	-128.84	-122.47	-157.79	-166.27	-131.37	*-151.60±3.5*
MoO3	-76.56	-69.88	-88.32	-68.24	-52.95	-57.22	-51.51	-74.37	-83.73	-54.99	*-86.70±5.0*
$MoOCl_4$	-137.99	-120.66	-149.65	-121.18	-120.61	-111.20	-103.84	-152.08	-153.14	-117.26	*-135.90±1.4*
NbO	52.07	54.09	49.59	54.71	60.31	57.88	59.97	47.78	54.58	53.65	*47.50±5.0*
NbO_2	-42.30	-37.89	-49.32	-36.78	-26.60	-29.95	-25.92	-47.25	-40.32	-32.50	*-47.80±5.0*
RhC	166.05	175.90	166.81	174.60	173.24	180.26	181.99	154.68	198.36	175.83	*164.10±2.3*
$RhCl_2$	29.52	44.94	33.01	44.14	39.83	46.91	49.50	28.48	40.28	46.03	*30.00±3.0*
RhO	90.94	95.34	90.06	96.25	98.46	101.25	103.12	82.49	115.12	101.65	*95.00±10.0*
RuO_4	-87.10	-66.28	-83.67	-62.22	-56.91	-42.47	-23.72	-59.58	-38.95	-9.71	*-46.03±1.0*
YO	-12.14	-5.31	-4.57	-4.56	-7.35	-1.18	0.01	0.63	2.57	-0.22	*-11.00±2.5*
ZrBr	70.57	84.73	72.61	78.74	80.62	85.91	87.15	78.89	90.17	84.86	*71.90±0.5*
$ZrBr_4$	-173.66	-153.44	-167.03	-154.71	-169.93	-149.95	-145.80	-156.90	-148.21	-151.80	*-166.00±2.0*

ZrCl	58.69	63.68	60.06	63.37	59.76	64.78	66.03	56.27	64.61	59.43	*67.59±5.7*
$ZrCl_2$	-15.17	-30.13	-32.19	-30.58	-40.53	-28.12	-26.35	-30.17	-30.34	-34.82	*-34.87±3.6*
$ZrCl_4$	-219.82	-200.00	-215.67	-201.18	-215.79	-196.17	-191.89	-220.34	-209.03	-208.47	*-208.03±0.6*
ZrO	20.45	26.19	23.91	26.81	27.17	31.18	32.95	18.41	37.90	29.57	*21.80*
ZrO_2	-78.84	-64.85	-71.07	-63.32	-66.50	-55.26	-52.38	-67.39	-44.60	-56.47	*-68.40±11.0*

Table 4S. The enthalpies of formation (ΔH_f's) for the TM-4*d* set as determined by the range-separated (RS) and range-separated hybrid (RSH) functionals. See Reference 2 for more details about the experimental data and uncertainties. Units are in kcal mol^{-1}.

Molecule	ωB97XD	ωB97X	CAM-B3LYP	ωB97	LC-ωPBE	Experiment
AgH	65.22	63.66	66.01	62.68	68.19	*66.30*
Cd_2	51.40	51.30	53.05	51.07	52.74	*51.40*
CdBr	19.85	19.66	18.76	20.09	11.74	*15.89*
$CdBr_2$	-35.59	-37.95	-33.30	-38.88	-43.23	*-33.45±1.1*
CdCl	13.18	12.78	12.97	12.80	4.72	*6.55*
$CdCl_2$	-50.25	-53.13	-46.08	-54.88	-57.81	*-46.50±1.1*
CdH	72.64	72.23	68.37	71.81	62.81	*62.30*
$MoCO_5$	-149.50	-149.76	-138.59	-153.80	-132.64	*-157.50±5.0*
$MoCO_6$	-209.59	-209.53	-198.62	-213.60	-194.74	*-218.95±1.1*
MoF	61.17	55.67	57.96	51.04	59.26	*67.60±3.0*
MoF_2	-24.31	-50.34	-28.43	-58.69	-43.81	*-38.90±4.0*
MoF_6	-385.25	-400.39	-391.69	-417.26	-382.37	*-372.30±2.2*
MoO_2	0.07	-5.80	2.59	-12.30	10.46	*-1.98±3.0*
MoO_2Cl_2	-149.21	-155.07	-136.17	-161.87	-126.20	*-151.60±3.5*
MoO_3	-73.04	-79.78	-66.37	-87.94	-57.22	*-86.70±5.0*
$MoOCl_4$	-133.15	-137.10	-114.45	-141.27	-102.72	*-135.90±1.4*
NbO	26.63	24.18	54.39	21.95	58.23	*47.50±5.0*
NbO_2	-67.11	-71.67	-36.13	-76.01	-28.43	*-47.80±5.0*
RhC	173.71	170.77	179.91	171.83	182.49	*164.10±2.3*
$RhCl_2$	36.73	29.06	43.84	30.21	44.07	*30.00±3.0*
RhO	94.61	88.68	97.35	88.47	96.80	*95.00±10.0*
RuO_4	-60.11	-55.33	-53.81	-54.58	-74.53	*-46.03±1.0*
YO	-3.90	-0.67	-5.95	0.08	-13.02	*-11.00±2.5*
ZrBr	70.87	71.40	72.77	71.58	82.54	*71.90±0.5*
$ZrBr_4$	-167.17	-163.35	-156.12	-160.24	-157.88	*-166.00±2.0*
ZrCl	67.27	57.59	70.01	66.73	60.02	*67.59±5.7*
$ZrCl_2$	-36.40	-33.69	-35.72	-31.29	-42.17	*-34.87±3.6*
$ZrCl_4$	-218.46	-217.07	-205.51	-216.07	-210.04	*-208.03±0.6*
ZrO	21.02	21.92	23.99	21.39	26.38	*21.80*
ZrO_2	-70.46	-67.87	-67.01	-68.55	-73.59	*-68.40±11.0*

Table 5S. The enthalpies of formation (ΔH_f's) for the TM-4*d* set as determined by the double hybrid (DH) functionals. See Reference 2 for more details about the experimental data and uncertainties. Units are in kcal mol^{-1}.

Molecule	mPW2-PLYP	B2GP-PLYP	Experiment
AgH	67.72	68.44	*66.30*
Cd_2	52.61	52.67	*51.40*
CdBr	18.20	17.78	*15.89*
$CdBr_2$	-35.48	-36.80	*-33.45±1.1*
CdCl	13.34	12.90	*6.55*
$CdCl_2$	-46.29	-47.47	*-46.50±1.1*
CdH	71.77	71.92	*62.30*
$MoCO_5$	-152.29	-154.43	*-157.50±5.0*
$MoCO_6$	-214.20	-217.54	*-218.95±1.1*
MoF	61.48	62.35	*67.60±3.0*
MoF_2	-40.33	-38.89	*-38.90±4.0*
MoF_6	-383.01	-380.25	*-372.30±2.2*
MoO_2	-5.50	-5.82	*-1.98±3.0*
MoO_2Cl_2	-152.89	-155.72	*-151.60±3.5*
MoO_3	-79.86	-82.02	*-86.70±5.0*
$MoOCl_4$	-134.61	-136.65	*-135.90±1.4*
NbO	50.70	50.53	*47.50±5.0*
NbO_2	-45.55	-46.73	*-47.80±5.0*
RhC	161.93	157.62	*164.10±2.3*
$RhCl_2$	44.64	46.26	*30.00±3.0*
RhO	94.43	116.59	*95.00±10.0*
RuO_4	-47.45	-68.61	*-46.03±1.0*
YO	-6.71	-7.34	*-11.00±2.5*
ZrBr	86.77	86.76	*71.90±0.5*
$ZrBr_4$	-162.50	-165.37	*-166.00±2.0*
ZrCl	66.34	66.71	*67.59±5.7*
$ZrCl_2$	-30.56	-31.69	*-34.87±3.6*
$ZrCl_4$	-205.45	-207.26	*-208.03±0.6*
ZrO	27.16	23.07	*21.80*
ZrO_2	-65.98	-71.18	*-68.40±11.0*

Table 6S. Ground state geometries for the TM-4*d* set as determined by B3LYP/cc-pVTZ-PP. Radii (r) are reported in Angstrom, bond angles (A) and dihedral angles (D) are reported in degrees.

Diatomic			**Tetrahedral**		
AgH	*r (Ag-H)*	1.619	**MoO_2Cl_2**	*r (Mo-O)*	1.677
Cd2	*r (Cd-Cd)*	4.077		*r (Mo-Cl)*	2.266
CdBr	*r (Cd-Br)*	2.537		*A (O-Mo-O)*	107.0
CdCl	*r (Cd-Cl)*	2.397		*A (Cl-Mo-Cl)*	111.4
CdH	*r (Cd-H)*	1.518		*A (O-Mo-Cl)*	109.6
MoF	*r (Mo-F)*	1.904	**RuO_4**	*r (Ru-O)*	1.682
NbO	*r (Nb-O)*	1.687		*A (O-Ru-O)*	109.5
RhC	*r (Rh-C)*	1.604	**$ZrBr_4$**	*r (Zr-Br)*	2.491
RhO	*r (Rh-O)*	1.709		*A (Br-Zr-Br)*	109.5
YO	*r (Y-O)*	1.802	**$ZrCl_4$**	*r (Zr-Cl)*	2.342
ZrBr	*r (Zr-Br)*	2.590		*A (Cl-Zr-Cl)*	109.5
ZrCl	*r (Zr-Cl)*	2.304			
ZrO	*r (Zr-O)*	1.857			
Linear			**Square pyramidal**		
$CdBr_2$	*r (Cd-Br)*	2.419	**$Mo(CO)_5$**	*r (Mo-C)*	1.950
	A (Br-Cd-Br)	180.0		*r (C-O)*	1.150
$CdCl_2$	*r (Cd-Cl)*	2.286		*A (C-Mo-C)*	89.8
	A (Cl-Cd-Cl)	180.0		*A (O-C-Mo)*	178.1
MoF_2	*r (Mo-F)*	1.904	**$MoOCl_4$**	*r (Mo-O)*	1.652
	A (F-Mo-F)	180.0		*r (Mo-Cl)*	2.304
$RhCl_2$	*r (Rh-Cl)*	2.211		*A (O-Mo-Cl)*	104.2
	A (Cl-Rh-Cl)	180.0		*A (Cl-Mo-Cl)*	86.6
				D (Cl-Mo-O-Cl)	90.0
Bent			**Octahedral**		
MoO_2	*r (Mo-O)*	1.699	**$Mo(CO)_6$**	*r (Mo-C)*	2.075
	A (O-Mo-O)	115.1		*r (C-O)*	1.140
NbO_2	*r (Nb-O)*	1.712		*A (C-Mo-C)*	90.0
	A (O-Nb-O)	105.4		*A (O-C-Mo)*	180.0
$ZrCl_2$	*r (Zr-Cl)*	2.378	**MoF6**	*r (Mo-F)*	1.834
	A (Cl-Zr-Cl)	154.5		*A (F-Mo-F)*	180.0
ZrO_2	*r (Zr-O)*	1.776			
	A (O-Zr-O)	108.5			
Triagonal pyramidal					
MoO_3	*r (Mo-O)*	1.713			
	A (O-Mo-O)	120.0			
	D (O-Mo-O-O)	180.0			

Table 7S. Experimental and previous theoretically-determined geometries for the diatomics of the TM-4*d* molecule set.

Diatomic	Experiment	Theory
AgH	1.618 [a]	1.5635 [b]
Cd_2	4.070 [c], 4.380 [d], 3.770 [e], 3.760 [f]	3.961 [g]
CdBr		2.563 [h], 2.466 [i]
CdCl		2.413 [h], 2.333 [i]
CdH	1.761 [j]	1.752 [i]
MoF		1.935 [h], 2.000 [h]
NbO	1.690 [k]	1.710 [m], 1.709 [n]
RhC	1.613 [a]	1.623 [p]
RhO		1.740 [m], 1.739 [n]
YO	1.790 [a]	1.820 [m], 1.830 [n]
ZrBr		2.463 [h]
ZrCl	2.284 [q]	2.351 [h]
ZrO	1.712 [k]	1.740 [m], 1.761 [n]

[a] From Ref. 3.
[b] From Ref. 4.
[c] From Ref. 5.
[d] From Ref. 6.
[e] From Ref. 7.
[f] From Ref. 8.
[g] From Ref. 9.
[h] From Ref. 10.
[i] From Ref. 11.
[j] From Ref. 12.
[k] From Ref. 13.
[m] From Ref. 14.
[n] From Ref. 15.
[p] From Ref. 16.
[q] From Ref. 17.

Table 8S. Experimental and previous theoretically-determined geometries for the tri- and tetra-atomics of the TM-4*d* molecule set.

Linear	Experiment	Theory	
$CdBr_2$	2.386 [a], 2.372 [b], 2.394 [c]	2.405 [d], 2.381 [d], 2.377 [d]	
$CdCl_2$	2.266 [a], 2.210 [c], 2.266 [f], 2.282 [g]	2.273 [d], 2.254 [d], 2.249 [d]	
Bent		**Theory**	
		r_e	**Angle**
MoO_2		1.720 [h]	132.2
NbO_2		1.740 [h]	111.8
ZrO_2		1.797 [i]	109.6
		1.816 [i]	109.4
		1.806 [i]	108.0
		1.780 [h]	112.3
Triagonal pyramidal		**Theory**	
		r_e	**Symmetry**
MoO_3		1.700 [h]	(C_{3v})

[a] From Ref. 18.
[b] From Ref. 19.
[c] From Ref. 20.
[d] From Ref. 21.
[f] From Ref. 22.
[g] From Ref. 23.
[h] From Ref. 24.
[i] From Ref. 25.

Table 9S. Experimental and previous theoretically-determined geometries for molecules with greater than 4 atoms from the 4d-TM molecule set.

Tetrahedral		**Experiment**	**Theory**
MoO_2Cl_2	Mo-O		1.698 [a]
	Mo-Cl		2.259 [a]
	∠OMCl		104 +/- 2 [a]
	∠ClMCl		112 [a]
$ZrBr_4$		2.465 [b]	2.525 [c], 2.556 [c]
$ZrCl_4$		2.323 [d], 2.328 [b]	2.302 [e], 2.369 [d], 2.396 [d]
Square pyramidal		**Experiment**	**Theory**[f]
$Mo(CO)_5$	$Mo\text{-}C_{ax}$		1.947
	$Mo\text{-}C_{eq}$		2.066
	$Co\text{-}O_{ax}$		1.197
	$Co\text{-}O_{eq}$		1.185
	$\angle C_{ax}MoC_{eq}$		88.2
Octahedral		**Experiment**	**Theory**
$Mo(CO)_6$	Mo-C	2.063 [g]	2.116 [f]
	C-O	1.145 [g]	1.136 [f]
	Mo-CO		2.064 [h]
	Mo-Cax		2.064 [h]
	Mo-Ceq		2.064 [h]
MoF_6		1.817 [i], 1.809 [j]	1.825 [k]

[a] From Ref. 26.
[b] From Ref. 27.
[c] From Ref. 28.
[d] From Ref. 29.
[e] From Ref. 30.
[f] From Ref. 31.
[g] From Ref. 32.
[h] From Ref. 33.
[i] From Ref. 34.
[j] From Ref. 35.
[k] From Ref. 36.

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