

A Combined Experimental and Theoretical Study of the $\text{Ti}_2 + \text{N}_2\text{O}$ Reaction

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SUPPLEMENTARY INFORMATION

The following table lists the calculated geometric and energetic parameters of the Ti₂O structure at its four possible spin states. The calculations are all done with all the DFT functionals used in this manuscript as implemented in Gaussian 09 employing the Pople 6-311+G(2d) basis set. The table lists as well the spin contamination of the singlet state.

Table S- 1. The optimized geometrical and energetic parameters of the four spin states of Ti₂O. The septet state is found to be stable in linear and bent forms. Absolute energies E are in Hartree, relative energies (Te) in kJ/mol, distances in Å and angles in degree.

		E	S ²	Te	<TiOTi>	O-Ti	Ti-Ti
BB95	sing	-1774.41081	0.6	-	69.215	1.849	2.1
	trip	-1774.410404		+1.07	70.16	1.849	2.126
	quint	-1774.40079		+26.30	81.16	1.84	2.394
	sept	-1774.37355		+97.83	89.67	1.835	2.588
	sept_lin	-1774.37057		+105.65	180	1.813	3.628
BP86	sing	-1774.353397	0.7	-	69.451	1.846	2.103
	trip	-1774.353393		+0.0184	70.272	1.847	2.126
	quint	-1774.34768		+15.01	81.29	1.838	2.394
	sept	-1774.32251		+81.10	91.66	1.832	2.628
	sept_lin	-1774.3199152		+87.91	180	1.814	3.629
M06L	sing	-1774.019972	0.7	-	69.637	1.844	2.106
	trip	-1774.017701		+5.96	70.828	1.845	2.138
	quint	-1774.01614		+10.06	81.19	1.838	2.393
	sept	-1773.97088		+128.89	92.113	1.836	2.644
	sept_lin	-1773.9701417		+130.82	180	1.817	3.636
mPWPW91	sing	-1774.278161	0.7	-	69.588	1.846	2.106
	trip	-1774.278334		-0.465	70.404	1.846	2.128
	quint	-1774.17586		+268.59	81.28	1.838	2.394
	sept	-1774.15112		+333.549	91.88	1.833	2.634
	sept_lin	-1774.1487381		+339.80	180	1.816	3.631

	sing	-1774.572726	0.6	-	69.034	1.828	2.072
	trip	-1774.572914		-0.48	70.318	1.827	2.104
OB95	quint	-1774.56444		+21.77	80.48	1.823	2.355
	sept	-1774.54314		+77.69	86.45	1.821	2.494
	sept_lin	-1774.53209		+106.71	180	1.797	3.594
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	sing	-1774.224437	0.7	-	69.252	1.828	2.072
	trip	-1774.224947		-1.33	70.485	1.827	2.104
OPBE	quint	-1774.2215		+7.73	80.44	1.82	2.351
	sept	-1774.20778		+43.75	87.8	1.818	2.52
	sept_lin	-1774.19765		+70.33	180	1.799	3.598
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	sing	-1774.182175	0.6	-	69.614	1.824	2.073
	trip	-1774.181896		+0.75	70.539	1.823	2.104
BLYP	quint	-1774.17561		+17.25	82.133	1.852	2.433
	sept	-1774.14336		+101.93	97.35	1.846	2.772
	sept_lin	-1774.14906		+86.97	180	1.833	3.667
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	sing	-1774.193327	0.7	-	69.548	1.846	2.106
	trip	-1774.193351		-0.055	70.285	1.846	2.126
TPSS	quint	-1774.18121		+31.81	81.09	1.84	2.393
	sept	-1774.1644		+75.97	93.2	1.835	2.667
	sept_lin	-1774.1678788		+66.82	180	1.815	3.629
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	sing	-1774.181087	0.7	-	69.598	1.844	2.105
	trip	-1774.181309		-0.58	70.344	1.845	2.125
PW91PW91	quint	-1774.17586		+13.73	81.32	1.836	2.393
	sept	-1774.15112		+78.68	91.64	1.831	2.626
	sept_lin	-1774.1487381		+84.94	180	1.814	3.627
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	sing	-1773.605635	0.7	-	69.589	1.845	2.106
	trip	-1773.605878		-0.65	70.309	1.846	2.125
PBEPBE	quint	-1773.60011		+14.51	81.317	1.837	2.394
	sept	-1773.57501		+80.40	91.51	1.832	2.624
	sept_lin	-1773.5723933		+87.26	180	1.814	3.629
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	sing	-1774.245649	0.7	-	69.575	1.846	2.107
BPW91	trip	-1774.24577		-0.31	70.44	1.847	2.13
	quint	-1774.24173		+10.29	81.23	1.838	2.394

sept	-1774.22269	+60.28	91.96	1.833	2.636
sept_lin	-1774.22061268	+65.74	180	1.816	3.633
