

Supporting Information for the Manuscript:

Relativistic GVVPT2 Multireference Perturbation Theory Description of the Electronic States of Y_2 and Tc_2

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Table 1. Data on state-averaged calculations of PECs of the lowest three $1^1\Sigma_g^+$ states of Y_2 using the aug-cc-pVTZ-DK basis set.

GVVPT2 Energies (a.u.)			Distance (Å)
$1^1\Sigma_g^+$	$2^1\Sigma_g^+$	$3^1\Sigma_g^+$	
-6766.21510861789	-6766.20924084774	-6766.18212353846	2.4
-6766.23488873532	-6766.22868970566	-6766.18741619181	2.5
-6766.25396288488	-6766.24626061611	-6766.20845418212	2.6
-6766.27266878966	-6766.26511615785	-6766.22990912921	2.7
-6766.28255362667	-6766.27491883165	-6766.24288526800	2.8
-6766.28962976186	-6766.28215457385	-6766.25247461728	2.9
-6766.29420783973	-6766.28705548413	-6766.25914739831	3

-6766.29670564957	-6766.28999221024	-6766.26349186284	3.1
-6766.29752438113	-6766.29128987735	-6766.26584525876	3.19
-6766.29754520837	-6766.29136881021	-6766.26603107659	3.2
-6766.29755374472	-6766.29143640015	-6766.26620278397	3.21
-6766.29755050137	-6766.29149309307	-6766.26636065673	3.22
-6766.29753580349	-6766.29153917150	-6766.26650510689	3.23
-6766.29750995427	-6766.29157492738	-6766.26663667349	3.24
-6766.29747324287	-6766.29160065622	-6766.26675584578	3.25
-6766.29742595185	-6766.29161664866	-6766.26686302116	3.26
-6766.29736846661	-6766.29162329370	-6766.26695862530	3.27
-6766.29730106650	-6766.29162086877	-6766.26704293272	3.28
-6766.29722419650	-6766.29160981251	-6766.26711636726	3.29
-6766.29713813436	-6766.29159039307	-6766.26717917891	3.3
-6766.29682834467	-6766.29148538230	-6766.26730723699	3.33
-6766.29670897068	-6766.29143583803	-6766.26733085392	3.34
-6766.29658207654	-6766.29137953266	-6766.26734546590	3.35
-6766.29644795853	-6766.29131674452	-6766.26735136230	3.36
-6766.29630693553	-6766.29124777269	-6766.26734885256	3.37
-6766.29615930808	-6766.29117289542	-6766.26733822218	3.38
-6766.29584549590	-6766.29100657785	-6766.26729376424	3.4
-6766.29397934849	-6766.28990858026	-6766.26667392188	3.5
-6766.29180969043	-6766.28852047082	-6766.26556152857	3.6
-6766.28737936596	-6766.28542784349	-6766.26262152036	3.8
-6766.28360049718	-6766.28248677116	-6766.25966764635	4
-6766.28051261872	-6766.27998914831	-6766.25799786419	4.2
-6766.27898357615	-6766.27883785126	-6766.25859374170	4.3
-6766.27793743714	-6766.27716305505	-6766.26156193663	4.4
-6766.27960166793	-6766.27491972638	-6766.26582733302	4.5
-6766.27823572730	-6766.27331905077	-6766.26733162878	4.6
-6766.27512206119	-6766.27212365871	-6766.26779138745	4.7
-6766.27484449099	-6766.27201465322	-6766.26779857120	4.71
-6766.27457389733	-6766.27190705579	-6766.26780126240	4.72
-6766.27431032808	-6766.27180083329	-6766.26779992148	4.73
-6766.27405383105	-6766.27169594209	-6766.26779492304	4.74
-6766.27266933780	-6766.27109516042	-6766.26770471887	4.8
-6766.26980452661	-6766.26948344199	-6766.26700495022	5
-6766.26839060585	-6766.26836711882	-6766.26614377613	5.2
-6766.26754951435	-6766.26750111802	-6766.26537514475	5.4
-6766.26691548923	-6766.26685281601	-6766.26475121779	5.6
-6766.26641332631	-6766.26635237248	-6766.26424366453	5.8
-6766.26600959188	-6766.26595493204	-6766.26383098900	6
-6766.26530905439	-6766.26527137446	-6766.26311172100	6.5
-6766.26489804652	-6766.26487269320	-6766.26267432931	7
-6766.26461293407	-6766.26459569163	-6766.26238229250	7.5
-6766.26437823180	-6766.26436627865	-6766.26217030506	8
-6766.26406454589	-6766.26405842770	-6766.26184939929	9

Table 2. Data on state-averaged calculations of PECs of the lowest three $1^1\Sigma_g^+$ states of Y_2 using the aug-cc-pVTZ-DK basis set and including $5p_z$ -derived MOs in the active space.

$1^1\Sigma_g^+$	GVVPT2 Energies (a.u.)			Distance (\AA)
	$2^1\Sigma_g^+$	$3^1\Sigma_g^+$		
-6766.211098376519	-6766.129836293774	-6766.115680613706	2	
-6766.280046452493	-6766.211488801789	-6766.203735096137	2.2	
-6766.302006009741	-6766.273723419432	-6766.260515692179	2.6	
-6766.303064805692	-6766.281183921605	-6766.274515254908	2.8	
-6766.297410345452	-6766.292532211200	-6766.275668836530	3	
-6766.300414323710	-6766.296345807032	-6766.284795075563	3.2	
-6766.298288592604	-6766.296956874732	-6766.287185353878	3.4	
-6766.295773252405	-6766.294263247501	-6766.286307264715	3.6	
-6766.294575163330	-6766.292269474568	-6766.285638608064	3.7	
-6766.293061145998	-6766.290518563271	-6766.284928912308	3.8	
-6766.289920013168	-6766.287521806833	-6766.282877545710	4	
-6766.288476185960	-6766.285968556105	-6766.281439245385	4.1	
-6766.287065454922	-6766.284338298692	-6766.279892814589	4.2	
-6766.285645414282	-6766.282723879714	-6766.278408527772	4.3	
-6766.284162534693	-6766.281206640874	-6766.277079278472	4.4	
-6766.280662061221	-6766.278595375645	-6766.274918548016	4.6	
-6766.277187991187	-6766.276511818068	-6766.273197098730	4.8	
-6766.274932824288	-6766.274841364136	-6766.271788277116	5	
-6766.273495959853	-6766.273446856194	-6766.270647540095	5.2	
-6766.272405527319	-6766.272333805974	-6766.269714603819	5.4	
-6766.271514234149	-6766.271446892553	-6766.268950498791	5.6	
-6766.270184415127	-6766.270135431793	-6766.267774878117	6	

Table 3. Data on the PEC of ground state Y_2 computed with the aug-cc-pVTZ-DK basis set.

$X^5\Sigma_u^-$	Distance (Å)
-6766.247065967779	2.2
-6766.293553339320	2.4
-6766.315939967324	2.6
-6766.322139619669	2.79
-6766.322159483067	2.8
-6766.322153699979	2.81
-6766.322122859071	2.82
-6766.322067677836	2.83
-6766.321988690833	2.84
-6766.321886600552	2.85
-6766.321049914122	2.9
-6766.317962780066	3
-6766.307727904154	3.2
-6766.294471231765	3.4
-6766.280352952548	3.6
-6766.273432107496	3.7
-6766.266728447256	3.8
-6766.260079257826	3.9
-6766.244859760510	4.1
-6766.240143614238	4.2
-6766.236307878899	4.3
-6766.232960554791	4.4
-6766.229873329570	4.5
-6766.227008511271	4.6
-6766.224395810576	4.7
-6766.222052993462	4.8
-6766.219980005046	4.9
-6766.218165812576	5
-6766.216592932433	5.1
-6766.215240227210	5.2
-6766.214084632922	5.3
-6766.213102402333	5.4
-6766.212270490997	5.5
-6766.211567263933	5.6
-6766.210469808869	5.8
-6766.209679783522	6
-6766.208678728779	6.4
-6766.208118879860	6.8
-6766.207775385050	7.2
-6766.207532703093	7.6
-6766.207343079294	8

Table 4. Data on PECs of the computed electronic states of Tc₂ using the aug-cc-pVTZ-DK basis set.

$X^3\Sigma_g^-$		$1^1\Sigma_g^+$		$1^5\Sigma_g^+$	
GVVPT2 Energy (a.u.)	Distance (Å)	GVVPT2 Energy (a.u.)	Distance (Å)	GVVPT2 Energy (a.u.)	Distance (Å)
-8567.00773007562	1.8	-8566.99926408425	1.8	-8566.90153386353	1.8
-8567.07539516369	2	-8567.03675662471	1.9	-8566.96629403232	1.9
-8567.08320789137	2.1	-8567.05612496641	2	-8567.00463215582	2
-8567.08355302806	2.12	-8567.06446486674	2.1	-8567.02656185648	2.1
-8567.08360497035	2.13	-8567.06630786627	2.18	-8567.03741947671	2.2
-8567.08348792648	2.15	-8567.06631898482	2.19	-8567.04056520209	2.3
-8567.08207526797	2.2	-8567.06628744972	2.2	-8567.04058750757	2.31
-8567.07562472788	2.3	-8567.06621467947	2.21	-8567.04056949729	2.32
-8567.04306718848	2.6	-8567.06390157066	2.3	-8567.04051396527	2.33
-8567.02455737574	2.8	-8567.05853932192	2.4	-8567.04042340365	2.34
-8567.01009117548	3	-8567.04328475486	2.6	-8567.03926473269	2.4
-8566.99790743191	3.2	-8567.02658637121	2.8	-8567.03074914158	2.6
-8566.97937133357	3.6	-8567.01033760158	3	-8567.02491852211	2.7
-8566.96802046678	4	-8566.99577510274	3.2	-8567.01840885715	2.8
-8566.96190972155	4.4	-8566.97846293176	3.5	-8567.01144316650	2.9
-8566.95879856908	4.8	-8566.96666570191	3.8	-8567.00432026121	3
-8566.95718855214	5.2	-8566.95941702024	4.1	-8566.99083715541	3.2
-8566.95631138883	5.6	-8566.95436593328	4.5	-8566.97948461403	3.4
-8566.95580620252	6	-8566.95206544078	4.9	-8566.97063567110	3.6
-8566.95525171327	7	-8566.95095452425	5.3	-8566.96412788566	3.8
-8566.95506246400	8	-8566.95035457950	5.7	-8566.95781427533	4.1
-8566.95497063586	9	-8566.95000043056	6.1	-8566.95426849259	4.4
-8566.95491096063	10	-8566.94962354796	7	-8566.95230177753	4.7
				-8566.95117693965	5
				-8566.95032409623	5.4
				-8566.94983330508	5.8
				-8566.94953199497	6.2
				-8566.94934347806	6.6
				-8566.94922486969	7
$1^9\Sigma_g^+$		$1^{11}\Sigma_g^-$			
-8566.92612224026	2.2	-8566.957052067819	2.12		
-8566.95841279588	2.3	-8566.967665790622	2.16		
-8566.97897450879	2.4	-8566.976079427011	2.2		
-8566.99118572868	2.5	-8566.982626952104	2.24		

-8566.99729977057	2.6	-8566.987594279915	2.28
-8566.99880926561	2.67	-8566.991227353707	2.32
-8566.99886616609	2.68	-8566.993739322263	2.36
-8566.99888584401	2.69	-8566.995315836410	2.4
-8566.99886898087	2.7	-8566.99621616883	2.45
-8566.99682998827	2.8	-8566.99627583110	2.46
-8566.98704419097	3	-8566.99630013052	2.47
-8566.97695488631	3.2	-8566.99629090166	2.48
-8566.96916997522	3.4	-8566.99625002706	2.49
-8566.96351171623	3.6	-8566.99617920629	2.5
-8566.95943395837	3.8	-8566.99417035804	2.6
-8566.95542360409	4.1	-8566.98663534163	2.8
-8566.95308469263	4.4	-8566.97877187287	3
-8566.95171857813	4.7	-8566.97240734312	3.2
-8566.95088335536	5	-8566.96767078605	3.4
-8566.95006558582	5.5	-8566.96292879920	3.7
-8566.94960024232	6	-8566.96010813233	4
-8566.94932711986	6.5	-8566.95807433210	4.4
-8566.94916914047	7	-8566.95700893198	4.8
		-8566.95634928957	5.2
		-8566.95588564740	5.6
		-8566.95555213085	6
		-8566.95527261683	6.5
		-8566.95509944528	7
		-8566.95491844542	8

Table 5. Data on PECs of the degenerate electronic states of Mn₂ (Shown in Figure 7 of the Manuscript) computed using the cc-pVTZ basis set.

GVVPT2 Energies (a.u.)			Distance (Å)
$1^1 \Sigma_g^+$	$1^5 \Sigma_g^+$	$1^9 \Sigma_g^+$	
-2300.67953915551	-2300.67946434779	-2300.67931084402	3.2
-2300.68034631101	-2300.68030237227	-2300.68021683654	3.3
-2300.68060609570	-2300.68057116161	-2300.68050524742	3.34
-2300.68083578194	-2300.68080836518	-2300.68075870678	3.38
-2300.68103861107	-2300.68101744790	-2300.68098119034	3.42
-2300.68121739519	-2300.68120141375	-2300.68117613690	3.46
-2300.68137458732	-2300.68136287773	-2300.68134653379	3.5
-2300.68151233909	-2300.68150413088	-2300.68149498989	3.54
-2300.68163255307	-2300.68162719618	-2300.68162380011	3.58
-2300.68173692678	-2300.68173387201	-2300.68173499521	3.62
-2300.68182698555	-2300.68182576971	-2300.68183038569	3.66
-2300.68190410549	-2300.68190434236	-2300.68191159367	3.7
-2300.68196953865	-2300.68197090333	-2300.68198007875	3.74
-2300.68202442432	-2300.68202664623	-2300.68203715732	3.78
-2300.68206979993	-2300.68207265570	-2300.68208401910	3.82
-2300.68210661269	-2300.68210991691	-2300.68212173868	3.86
-2300.68213572299	-2300.68213932365	-2300.68215128607	3.9
-2300.68215791180	-2300.68216168622	-2300.68217353475	3.94
-2300.68217388890	-2300.68217773704	-2300.68218927138	3.98
-2300.68218429440	-2300.68218813638	-2300.68219920180	4.02
-2300.68218970724	-2300.68219348011	-2300.68220395883	4.06
-2300.68219064760	-2300.68219430327	-2300.68220410993	4.1
-2300.68218758604	-2300.68219108794	-2300.68220016259	4.14
-2300.68218094628	-2300.68218426729	-2300.68219257204	4.18
-2300.68217111020	-2300.68217423145	-2300.68218174565	4.22
-2300.68215842385	-2300.68216133323	-2300.68216805084	4.26
-2300.68212572696	-2300.68212819663	-2300.68213334478	4.34
-2300.68208504811	-2300.68208708224	-2300.68209074445	4.42
-2300.68202575892	-2300.68202728396	-2300.68202926154	4.52
-2300.68197345881	-2300.68197461795	-2300.68197540746	4.6
-2300.68190414547	-2300.68190490663	-2300.68190441733	4.7
-2300.68183246268	-2300.68183289297	-2300.68183134550	4.8
-2300.68176020261	-2300.68176036514	-2300.68175796101	4.9
-2300.68168881367	-2300.68168876508	-2300.68168568120	5
-2300.68155289371	-2300.68155256170	-2300.68154854490	5.2
-2300.68143050903	-2300.68143002868	-2300.68142549053	5.4
-2300.68132392183	-2300.68132337838	-2300.68131858040	5.6
-2300.68123296741	-2300.68123241019	-2300.68122750781	5.8
-2300.68115610585	-2300.68115556017	-2300.68115063327	6

-2300.68109126807	-2300.68109074406	-2300.68108581956	6.2
-2300.68103641745	-2300.68103592000	-2300.68103104336	6.4
-2300.68098979780	-2300.68098932538	-2300.68098449854	6.6
-2300.68095000234	-2300.68094955139	-2300.68094476734	6.8
-2300.68091592153	-2300.68091548798	-2300.68091073833	7
-2300.68086152331	-2300.68086111342	-2300.68085640844	7.4
-2300.68080527133	-2300.68080487744	-2300.68080019508	8
-2300.68075433421	-2300.68075394505	-2300.68074924727	9
-2300.68073338927	-2300.68073299977	-2300.68072828895	10
