Theoretical study of the spectroscopy and radiative transition probabilities of Si$_2$ from visible to infrared

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Table S1. The dissociation limits relationship of the Λ-S states of Sn$_2$.

Atomic state (Si + Si)	Λ-S state	Relative Energy/cm^{-1}	
		This work	Expt.[34]
$^3P+^3P$	$^1\Sigma_g^+$(2), $^1\Sigma_u^-$, $^1\Pi_g$, $^1\Pi_u$, $^1\Delta_g$, $^3\Sigma_u^+$(2), $^3\Sigma_g^-$, $^3\Pi_g$, $^3\Pi_u$, $^3\Delta_u$, $^5\Sigma_g^+$(2), $^5\Sigma_u^-$, $^5\Pi_g$, $^5\Pi_u$, $^5\Delta_g$	0	0
$^3P+^1D$	$^3\Sigma_g^+$, $^3\Sigma_u^+$, $^3\Sigma_g^-$(2), $^3\Sigma_u^-$(2), $^3\Pi_g$(3), $^3\Pi_u$(3), $^3\Delta_g$(2), $^3\Delta_u$(2), $^3\Phi_g$, $^3\Phi_u$	6459.2	6298.9
$^1D+^1D$	$^1\Sigma_g^+$(3), $^1\Sigma_u^-$(2), $^1\Pi_g$(2), $^1\Pi_u$(2), $^1\Delta_g$(2), $^1\Delta_u$, $^1\Phi_g$, $^1\Phi_u$, $^1\Gamma_g$	12889.4	12448.0
$^3P+^1S$	$^3\Sigma_g^-$, $^3\Sigma_u^-$, $^3\Pi_g$, $^3\Pi_u$	14941.1	15394.4
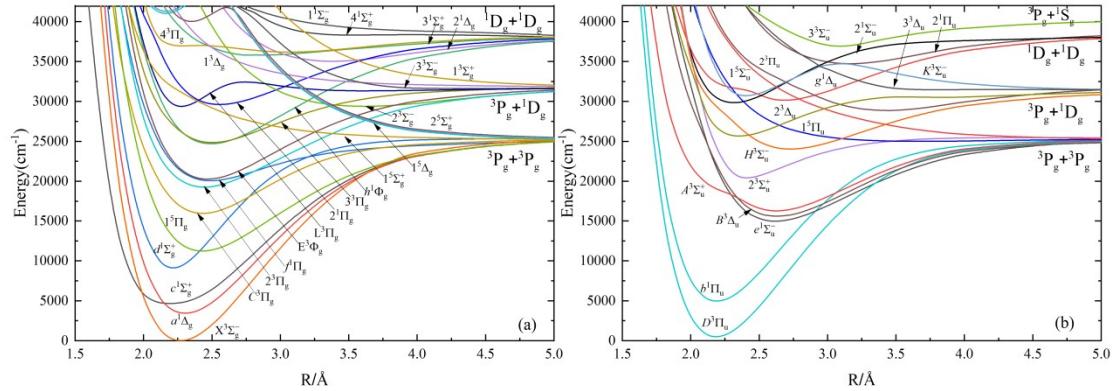
Figure S1 Potentials curves of the Λ-S electronic states of Si$_2$ as a function of internuclear separation R. (a) Symmetry g; (b) symmetry u.

Table S2. Spectroscopic constants of the triplet Λ-S states for Si$_2$

State		$\omega_e\chi_e$(cm^{-1})	B_e(cm^{-1})	Configuration (%)
X$^3\Sigma_g^-$	This work	2.0029	0.2337	3s$\sigma_g^2$3s$\sigma_u^2$3p$\sigma_g^2$3pπ_u^2 (83.5)
	Exp[10]	2.02	0.2390	
	Exp[12]	2.0085	0.23906	
	Cal[37]	2.15		
	Cal[24]	2.29	0.2360	
D$^3\Pi_u$	This work	2.1151	0.2529	3s$\sigma_g^2$3s$\sigma_u^2$3p$\sigma_g^1$3pπ_u^3 (80.3)
	Exp[9]	2.43	0.2596	

	Cal[37]	2.13		
	Cal[24]	2.51	0.2530	
$B^3\Delta_u$	This work	2.0423	0.1752	$3s\sigma_g^23s\sigma_u^23p\sigma_g^23p\pi_u^13p\pi_g^1$(83.1)
$C^3\Pi_g$	This work	2.5688	0.2040	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^1$ (80.8)
$A^3\Sigma_u^+$	This work	4.7270	0.1750	$3s\sigma_g^23s\sigma_u^23p\sigma_g^23p\pi_u^13p\pi_g^1$ (78.7)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^33p\pi_g^1$ (5.7)
$2^3\Pi_g$	This work	2.4646	0.2025	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^1$ (80.0)
$E^3\Phi_g$	This work	2.2776	0.1986	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^1$ (84.5)
$2^3\Sigma_u^+$	This work	10.4332	0.2087	$3s\sigma_g^23s\sigma_u^23p\sigma_g^23p\pi_u^13p\pi_g^1$ (21.9)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^33p\pi_g^1$ (50.1)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^13p\pi_g^3$ (5.6)
$H^3\Sigma_u^-$	This work	2.1621	0.1659	$3s\sigma_g^23s\sigma_u^23p\sigma_g^23p\pi_u^13p\pi_g^1$ (60.3)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^33p\pi_g^1$ (6.9)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^03p\sigma_u^1$ (12.5)
	Exp[9, 10]	1.99	0.1699	
	Exp[12]	1.64	0.17232	
$3^3\Pi_g$	This work	3.2175	0.1929	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^1$ (78.7)
$2^3\Delta_u$	This work	4.9558	0.2182	$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^33p\pi_g^1$ (75.1)
$2^3\Pi_u$	This work	1.7191	0.1022	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^13p\pi_g^2$(55.47)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^23p\pi_g^13p\sigma_u^1$(21.19)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^3$ (9.06)
$2^3\Sigma_g^-$	This work	0.9477	0.0917	$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^23p\pi_g^2$ (83.1)
$L^3\Pi_g$	This work	13.5756	0.2332	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^1$ (53.3)
				$3s\sigma_g^23s\sigma_u^13p\sigma_g^23p\pi_u^3$ (27.5)
	Exp [9]		0.2370	
$K^3\Sigma_u^-$	This work	6.8736	0.2098	$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^33p\pi_g^1$ (59.0)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^23p\pi_u^13p\pi_g^1$ (15.8)
	Exp[10]	5.95	0.2185	
$3^3\Sigma_u^-$	This work	6.9775	0.1267	$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^33p\pi_g^1$ (34.2)

$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^2 3p\pi_g^0 3p\sigma_u^1$(29.7)

$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^0 3p\pi_g^2 3p\sigma_u^1$(7.3)

$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^2 3p\pi_u^1 3p\pi_g^1$ (6.1)

$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^0 3p\pi_u^1 3p\pi_g^3$ (5.7)
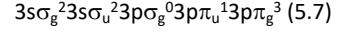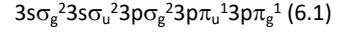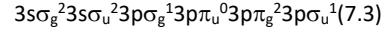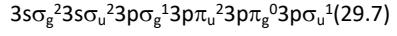
Table S3. Spectroscopic constants of the singlet Λ-S states for Si_2

| State		$\omega_e\chi_e$(cm^{-1})	B_e(cm^{-1})	Configuration (%)
$a^1\Delta_g$	This work	1.7426	0.2269	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^2 3p\pi_u^2$(81.7)
$c^1\Sigma^+g$	This work	-3.4564	0.2511	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^0 3p\pi_u^4$ (41.2)
				$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^2 3p\pi_u^2$ (37.1)
$b^1\Pi_u$	This work	2.2267	0.2517	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^3$ (80.1)
	Exp[18]	2.6123	0.2593	
$d^1\Sigma^+g$	This work	6.1160	0.2457	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^2 3p\pi_u^2$ (42.9)
				$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^0 3p\pi_u^4$ (31.5)
	Exp[18]	10.0232	0.251823	
$e^1\Sigma^-_u$	This work	2.0973	0.1760	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^2 3p\pi_u^1 3p\pi_g^1$(83.4)
$f^1\Pi_g$	This work	4.6496	0.1951	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^2 3p\pi_g^1$ (80.8)
$h^1\Phi_g$	This work	2.0312	0.1944	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^2 3p\pi_g^1$ (83.4)
$g^1\Delta_u$	This work	3.2751	0.1717	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^0 3p\pi_u^3 3p\pi_g^1$ (77.9)
$2^1\Pi_g$	This work	2.5515	0.1846	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^2 3p\pi_g^1$(74.65)
$2^1\Sigma^-_u$	This work	3.4417	0.2251	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^2 3p\pi_g^1$ (79.6)
$2^1\Pi_u$	This work	1.6952	0.1204	$3s\sigma_g^2 3s\sigma_u^2 3p\sigma_g^1 3p\pi_u^1 3p\pi_g^2$(60.0)
				$3s\sigma_g^2 3s\sigma_u^1 3p\sigma_g^2 3p\pi_u^2 3p\pi_g^1$(22.61)
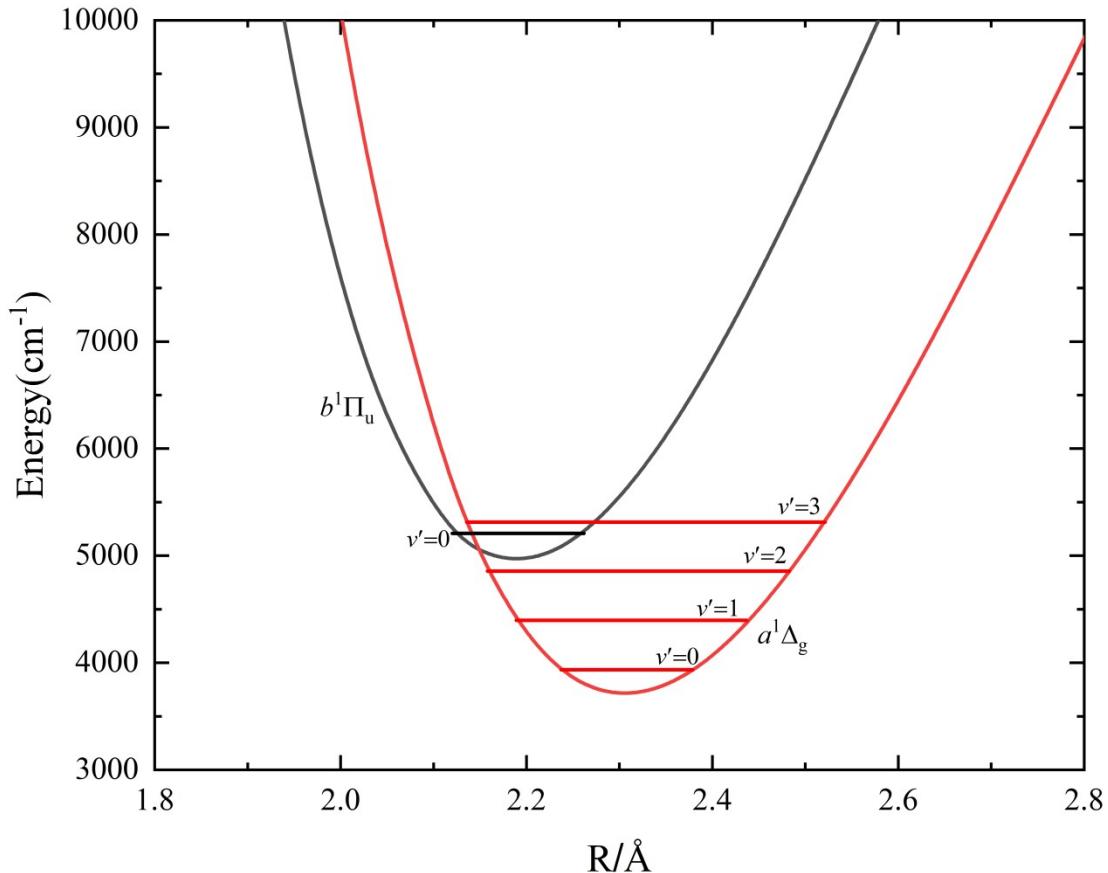
Figure S2. Potential energy curves with vibration energy level of $a^1\Delta_g$ and $b^1\Pi_u$ states.

Table S4. Spectroscopic constants of the quintet Λ-S states for Si_2

State		$\omega_e\chi_e$(cm^{-1})	B_e(cm^{-1})	Configuration (%)
$1^5\Pi_g$	This work	2.1239	0.2046	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^1$ (85.0)
$1^5\Pi_u$	This work	1.7908	0.0888	$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^13p\pi_g^2$ (62.9)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^23p\pi_g^13p\sigma_u^1$ (24.4)
$1^5\Sigma_g^+$	This work			$3s\sigma_g^2\,3s\sigma_u^23p\sigma_g^13p\pi_u^13p\pi_g^13p\sigma_u^1$ (57.2)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^23p\pi_g^2$ (30.4)
$1^5\Sigma_u^-$	This work			$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^23p\pi_g^03p\sigma_u^1$ (45.2)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^13p\pi_u^03p\pi_g^23p\sigma_u^1$ (42.4)
$1^5\Delta_g$	This work	12.1457	0.2576	$3s\sigma_g^23s\sigma_u^13p\sigma_g^13p\pi_u^33p\pi_g^1$ (82.6)
$2^5\Sigma_g^+$	This work	16.1514	0.2190	$3s\sigma_g^23s\sigma_u^13p\sigma_g^13p\pi_u^33p\pi_g^1$ (55.7)
				$3s\sigma_g^23s\sigma_u^23p\sigma_g^03p\pi_u^23p\pi_g^2$ (22.5)

Table S5. The electric dipole transition moment for the triplet-triplet transitions of Si$_2$. (a.u.)

R/Å	$X^3\Sigma^-_g$-$D^3\Pi_u$	$X^3\Sigma^-_g$-$2^3\Pi_u$	$D^3\Pi_u$-$C^3\Pi_g$	$D^3\Pi_u$-$2^3\Pi_g$	$D^3\Pi_u$-$L^3\Pi_g$	$D^3\Pi_u$-$3^3\Pi_g$	$D^3\Pi_u$-$2^3\Sigma^-_g$	$B^3\Delta_u$-$2^3\Pi_g$
1.9	0.35200	0.31871	0.46150	-0.13906	0.03532	0.03214	0.11584	-0.15817
1.95	0.34536	0.31263	0.36582	-0.16371	0.04229	0.01811	0.08415	-0.13632
2	0.33711	0.30372	0.26993	-0.18160	0.04591	-0.00253	0.02736	-0.10013
2.05	0.32828	0.29320	0.17703	-0.18510	0.04301	-0.03229	-0.04462	-0.03790
2.11	0.31659	0.27887	0.08089	-0.16947	0.02252	-0.08127	-0.10447	0.06511
2.15	0.30818	0.26862	0.02853	-0.15230	-0.00907	-0.11823	-0.12276	0.11948
2.2	0.29746	0.25552	-0.02570	-0.12987	-0.07322	-0.15813	-0.12967	0.15730
2.25	0.28607	0.24190	-0.07142	-0.10859	-0.15800	-0.18562	-0.12631	0.17440
2.3	0.27568	0.22802	-0.11047	-0.09133	-0.24751	-0.20280	-0.09711	0.18074
2.35	0.26389	0.21410	-0.14557	-0.07720	-0.33793	-0.21666	-0.08194	0.18147
2.4	0.25188	0.20016	-0.17798	-0.06515	-0.43163	-0.23022	-0.06184	0.17883
2.45	0.23962	0.18618	-0.20853	-0.05444	-0.52558	-0.24380	-0.04511	0.17395
2.5	0.22760	0.17244	-0.23790	-0.04463	-0.61757	-0.25780	-0.03315	0.16779
2.55	0.21521	0.15863	-0.26625	-0.03492	-0.70021	-0.27189	-0.02505	0.16035
2.6	0.20290	0.14466	-0.29376	-0.02489	-0.76493	-0.28594	-0.01936	0.15219
2.65	0.19111	0.13007	-0.32076	-0.01363	-0.80107	-0.29955	-0.01549	0.14394
2.7	0.17916	0.11064	-0.34631	-0.00135	-0.80764	-0.31250	-0.01222	0.13495
2.75	0.16777	0.07984	-0.37186	0.01396	-0.78490	-0.32382	-0.00932	0.12593
2.82	0.15275	0.04389	-0.40731	0.03556	-0.72625	-0.33731	-0.00581	0.11395
2.84	0.14840	0.03828	-0.41631	0.04147	-0.70876	-0.34068	-0.00492	0.11026
2.88	0.13995	0.03046	-0.43303	0.05379	-0.67296	-0.34672	-0.00339	0.10291
2.9	0.13586	0.02767	-0.44073	0.06024	-0.65498	-0.34937	-0.00274	0.09926
2.95	0.12600	0.02259	-0.45794	0.07725	-0.61058	-0.35477	-0.00146	0.09026
3.01	0.11484	0.01855	-0.47451	0.09919	-0.55917	-0.35874	-0.00054	0.07976
3.05	0.10779	0.01655	-0.48291	0.11446	-0.52622	-0.35970	-0.00026	0.07298
3.1	0.09945	0.01450	-0.49034	0.13375	-0.48652	-0.35887	-0.00029	0.06479

R/Å	$H^3\Sigma^-_u$-$2^3\Pi_g$	$H^3\Sigma^-_u$-$C^3\Pi_g$	R/Å	$K^3\Sigma^-_u$-$2^3\Pi_g$	$K^3\Sigma^-_u$-$C^3\Pi_g$	$K^3\Sigma^-_u$-$L^3\Pi_g$	$3^3\Sigma^-_u$-$2^3\Pi_g$	$3^3\Sigma^-_u$-$C^3\Pi_g$
1.9	0.05714	0.29650	1.9	0.09648	-0.30833	-0.08684	-0.48221	-0.16350
1.95	0.09679	0.29452	1.95	-0.01866	-0.34055	-0.05319	-0.47239	-0.05599
2	0.13412	0.28778	2	-0.09850	-0.34425	-0.03552	-0.44497	0.02864
2.05	0.16968	0.27275	2.05	-0.16679	-0.33326	-0.02310	-0.40855	0.09817
2.11	0.18537	0.25854	2.11	-0.23186	-0.31046	-0.00872	-0.36189	0.15314
2.15	0.19494	0.23590	2.15	-0.26387	-0.29509	0.00269	-0.33476	0.17109
2.2	0.18835	0.20162	2.2	-0.29355	-0.27848	0.01810	-0.30498	0.18383
2.25	0.15333	0.14657	2.25	-0.30906	-0.25959	0.03489	-0.28469	0.17716
2.3	0.06914	0.05234	2.3	-0.30781	-0.23499	0.04715	-0.26706	0.16360
2.35	-0.02646	-0.03937	2.35	-0.29484	-0.20879	0.05504	-0.25037	0.14739
2.4	-0.07577	-0.08083	2.4	-0.27860	-0.18597	0.06151	-0.23432	0.13111
2.45	-0.09670	-0.09496	2.45	-0.26268	-0.16722	0.06803	-0.21928	0.11609
2.5	-0.10387	-0.09639	2.5	-0.24767	-0.15162	0.07486	-0.20563	0.10286
2.55	-0.10525	-0.09276	2.55	-0.23341	-0.13823	0.08165	-0.19364	0.09148
2.6	-0.10334	-0.08668	2.6	-0.21965	-0.12644	0.08745	-0.18339	0.08181

2.65	-0.10073	-0.07966		2.65	-0.20617	-0.11592	0.09080	-0.17483	0.07356
2.7	-0.09850	-0.07281		2.7	-0.19270	-0.10651	0.09035	-0.16783	0.06642
2.75	-0.09568	-0.06656		2.75	-0.17889	-0.09806	0.08596	-0.16218	0.06019
2.8	-0.09208	-0.06136		2.79	-0.16737	-0.09191	0.08014	-0.15858	0.05571
2.82	-0.09050	-0.05823		2.82	-0.15833	-0.08766	0.07470	-0.15641	0.05257
2.84	-0.08890	-0.05512		2.84	-0.15206	-0.08500	0.07061	-0.15522	0.05054
2.86	-0.08726	-0.05205		2.88	-0.13878	-0.08014	0.06136	-0.15349	0.04653
2.88	-0.08559	-0.04902		2.9	-0.13168	-0.07796	0.05616	-0.15294	0.04450
2.9	-0.08130	-0.04173		2.95	-0.11225	-0.07331	0.04128	-0.15237	0.03915
2.95	-0.07593	-0.03371		3.01	-0.08525	-0.06922	0.01956	-0.15234	0.03185
3	-0.07224	-0.02890		3.05	-0.06555	-0.06715	0.00332	-0.15145	0.02649
3.05	-0.06755	-0.02359		3.1	-0.04157	-0.06476	-0.01667	-0.14769	0.01998
3.1	-0.06284	-0.01905		3.2	-0.00766	-0.05933	-0.04550	-0.13134	0.01105

$R/\text{Å}$	$B^3\Delta_u-E^3\Phi_g$	$B^3\Delta_u-3^3\Pi_g$	$B^3\Delta_u-L^3\Pi_g$	$A^3\Sigma^+_u -2^3\Pi_g$	$A^3\Sigma^+_u - L^3\Pi_g$	$A^3\Sigma^+_u-3^3\Pi_g$	$X^3\Sigma^-_g - H^3\Sigma^-_u$
1.9	0.15689	0.12253	-0.18413	-0.23403	0.10138	-0.03625	-0.25290
1.95	0.13459	0.08798	-0.19284	-0.25010	0.10017	-0.04226	-0.26130
2	0.09804	0.03968	-0.20305	-0.25638	0.09798	-0.04949	-0.27099
2.05	0.02568	-0.03679	-0.21255	-0.24806	0.09694	-0.05731	-0.28218
2.11	-0.06595	-0.11273	-0.20305	-0.22122	0.09605	-0.06845	-0.30236
2.15	-0.12110	-0.15377	-0.17645	-0.19593	0.09414	-0.08116	-0.32580
2.2	-0.15964	-0.18059	-0.13490	-0.15581	0.09015	-0.10421	-0.37864
2.25	-0.17708	-0.18709	-0.10096	-0.09977	0.08868	-0.13302	-0.48271
2.3	-0.18363	-0.18288	-0.08073	-0.02407	0.09223	-0.16589	-0.64102
2.35	-0.18458	-0.17432	-0.06988	0.05615	0.09350	-0.19301	-0.78702
2.4	-0.18211	-0.16417	-0.06411	0.11104	0.06499	-0.20503	-0.86302
2.45	-0.17731	-0.15328	-0.06076	0.13735	0.06146	-0.20567	-0.88505
2.5	-0.17119	-0.14241	-0.05751	0.14680	0.05808	-0.20103	-0.88672
2.55	-0.16370	-0.13125	-0.05313	0.14668	0.05367	-0.19326	-0.87686
2.6	-0.15541	-0.12019	-0.04654	0.14149	0.04722	-0.18393	-0.86198
2.65	-0.14697	-0.10973	-0.03793	0.13371	0.03886	-0.17430	-0.84099
2.7	-0.13773	-0.09904	-0.02712	0.12396	0.02828	-0.16329	-0.82096
2.75	-0.12850	-0.08875	-0.01565	0.11356	0.01687	-0.15203	-0.79568
2.79	-0.12084	-0.08054	-0.00736	0.10466	0.00853	-0.14250	-0.77782
2.82	-0.11633	-0.07579	-0.00317	0.09884	0.00420	-0.13724	-0.76036
2.84	-0.11258	-0.07189	0.00014	0.09434	-0.00082	-0.13248	-0.75120
2.88	-0.10512	-0.06428	0.00607	0.08539	-0.00526	-0.12290	-0.73253
2.9	-0.10142	-0.06058	0.00872	0.08096	-0.00798	-0.11811	-0.72303
2.95	-0.09232	-0.05167	0.01453	0.07012	-0.01397	-0.10615	-0.69882
3.01	-0.08171	-0.04168	0.02023	0.05775	-0.01988	-0.09200	-0.66893
3.05	-0.07486	-0.03548	0.02341	0.05003	-0.02317	-0.08277	-0.64850
3.1	-0.06660	-0.02830	0.02682	0.04108	-0.02670	-0.07154	-0.62239

$R/\text{Å}$	$2^3\Sigma^-_g -2^3\Pi_u$	$2^3\Sigma^-_g - H^3\Sigma^-_u$	$3^3\Pi_g - 2^3\Sigma^+_u$	$L^3\Pi_g -2^3\Sigma^+_u$	$L^3\Pi_g - 2^3\Delta_u$	$2^3\Delta_u -2^3\Pi_g$	$2^3\Pi_u -C^3\Pi_g$
1.9	0.30629	-0.00308	0.14264	0.05409	-0.20628	0.47970	-0.41893
1.95	0.31892	0.07504	0.08885	0.11199	-0.15895	0.36925	-0.38750

R/Å	$a^1\Delta_g$-$b^1\Pi_u$	$b^1\Pi_u$-$f^1\Pi_g$	$b^1\Pi_u$-$2^1\Pi_g$	$c^1\Sigma_g^+$ - $b^1\Pi_u$	$a^1\Delta_g$ -$2^1\Pi_u$	$a^1\Delta_g$ -$g^1\Delta_u$	$a^1\Delta_g$ -$2^1\Pi_u$
2	0.31779	0.14077	-0.06096	0.35185	-0.07592	0.27782	-0.33119
2.05	0.29921	0.17814	-0.14030	0.37828	-0.03817	0.19988	-0.24348
2.11	0.28286	0.18213	-0.19765	0.34757	0.07590	0.16616	-0.17656
2.15	0.26157	0.17059	-0.24968	0.29655	0.08431	0.14143	-0.08612
2.2	0.23854	0.13723	-0.27566	0.24817	0.07312	0.13192	-0.01182
2.25	0.21070	0.06638	-0.28433	0.20706	0.05729	0.13269	0.10322
2.3	0.17537	-0.08826	-0.27858	0.17283	0.04064	0.14222	0.19149
2.35	0.12647	-0.32083	-0.25458	0.14400	0.02518	0.15396	0.27322
2.4	0.06262	-0.56482	-0.20806	0.11889	0.01089	0.16706	0.34857
2.45	0.01170	-0.81948	-0.14704	0.09853	-0.00238	0.17843	0.41973
2.5	-0.07013	-1.00373	-0.09879	0.08626	-0.01482	0.18382	0.48462
2.55	-0.10236	-1.10866	-0.06826	0.08039	-0.02629	0.17425	0.54536
2.6	-0.11045	-1.15111	-0.04995	0.07663	-0.03593	0.13185	0.60575
2.65	-0.08995	-1.16847	-0.03817	0.07389	-0.04375	-0.00504	0.65818
2.7	-0.03221	-1.15751	-0.02997	0.07052	-0.04933	-0.26964	0.65265
2.75	0.01192	-1.14858	-0.02558	0.06688	-0.05165	-0.42744	0.59424
2.8	0.03366	-1.13091	-0.02332	0.06152	-0.05064	-0.49045	0.54586
2.82	0.04224	-1.12287	-0.02193	0.05929	-0.05080	-0.50448	0.52355
2.84	0.04839	-1.11401	-0.02071	0.05705	-0.05078	-0.50905	0.50507
2.86	0.05284	-1.10440	-0.01964	0.05483	-0.05060	-0.50741	0.48944
2.88	0.05605	-1.09415	-0.01868	0.05263	-0.05029	-0.50165	0.47585
2.9	0.06063	-1.06608	-0.01669	0.04733	-0.04909	-0.47706	0.44703
2.95	0.06232	-1.02871	-0.01483	0.04141	-0.04703	-0.43979	0.41603
3	0.06214	-1.00205	-0.01379	0.03777	-0.04538	-0.41456	0.39518
3.05	0.06101	-0.96722	-0.01262	0.03358	-0.04309	-0.38512	0.36776
3.1	0.05919	-0.93115	-0.01154	0.02977	-0.04057	-0.35932	0.33855

R/Å	$a^1\Delta_g$-$b^1\Pi_u$	$b^1\Pi_u$-$f^1\Pi_g$	$b^1\Pi_u$-$2^1\Pi_g$	$c^1\Sigma_g^+$ - $b^1\Pi_u$	$a^1\Delta_g$ -$2^1\Pi_u$	$a^1\Delta_g$ -$g^1\Delta_u$	$a^1\Delta_g$ -$2^1\Pi_u$
1.85	-0.37156	0.58243	0.00277	-0.37325	-0.00119	-0.20269	0.26424
1.90	-0.36607	0.50752	-0.00129	-0.35295	-0.01355	-0.20706	0.25220
1.95	-0.35996	0.44156	-0.00244	-0.32837	-0.02473	-0.20935	0.23656
2.00	-0.35165	0.39056	-0.00274	-0.29744	-0.00488	-0.21788	0.38512
2.05	-0.34343	0.35277	-0.00296	-0.25599	-0.00527	-0.22836	0.36345
2.11	-0.33207	0.32198	-0.00288	-0.19092	-0.00583	-0.24769	0.33829
2.15	-0.32386	0.30866	-0.00271	-0.13729	-0.00640	-0.26634	0.32225
2.20	-0.31382	0.30052	-0.00250	-0.06480	-0.11606	-0.30022	0.06772
2.25	-0.30250	0.29527	-0.00216	0.00233	-0.09199	-0.35332	0.06751
2.30	-0.29088	0.29558	-0.00181	0.05321	-0.07182	-0.42413	0.06471
2.35	-0.27893	0.29935	-0.00143	0.08803	-0.05473	-0.50758	0.06031
2.40	-0.26641	0.30594	-0.00106	0.10996	-0.04122	-0.58135	0.05580
2.45	-0.25350	0.31452	0.00070	0.12346	-0.03009	-0.62642	0.05142
2.50	-0.24076	0.32498	0.00034	0.12955	-0.02137	-0.64645	0.04780
2.55	-0.22756	0.33667	0.00001	0.13104	-0.01444	-0.64585	0.04471
2.60	-0.21438	0.34943	0.00035	0.12952	-0.00882	-0.63350	0.04209
2.65	-0.20172	0.36262	0.00057	0.12624	-0.00414	-0.61045	0.03994

2.70	-0.18883	0.37638	0.00080	0.12114	0.00043	-0.58619	0.03799
2.75	-0.17650	0.38916	0.00084	0.11527	0.00260	-0.55484	0.03629
2.80	-0.16409	0.40248	0.00091	0.10891	0.00496	-0.52592	0.03488
2.82	-0.16033	0.40721	0.00085	0.10678	0.00586	-0.50983	0.03437
2.84	-0.15559	0.41223	0.00086	0.10387	0.00658	-0.49799	0.03380
2.86	-0.15092	0.41708	0.00086	0.10092	0.00722	-0.48603	0.03323
2.88	-0.14632	0.42174	0.00087	0.09794	0.00778	-0.47398	0.03267
2.90	-0.14179	0.42618	0.00086	0.09495	0.00827	-0.46186	0.03210
2.95	-0.13078	0.43617	0.00083	0.08744	0.00917	-0.43140	0.03065
3.00	-0.12028	0.44427	0.00079	0.08000	0.00966	-0.40091	0.02914

R/Å	$1^5\Pi_g$-$1^5\Pi_u$	R/Å	$K^3\Sigma_u^-$ -$X^3\Sigma_g^-$	$3^3\Sigma_u^-$ $X^3\Sigma_g^-$	R/Å	$2^3\Sigma_g^-$-$3^3\Sigma_u^-$
1.85	0.82990	1.9	-0.36251	1.58827	1.9	0.04723
1.9	0.73820	1.95	-0.79922	1.52428	1.95	0.03513
1.95	0.62870	2	-0.93344	1.47357	2	0.02817
2	0.51248	2.05	-0.97401	1.42181	2.05	0.02225
2.05	0.38670	2.11	-0.96466	1.32919	2.11	0.02416
2.11	0.22826	2.15	-0.93295	1.23909	2.15	0.03009
2.15	0.12002	2.2	-0.87283	1.13816	2.2	0.01908
2.2	0.01621	2.25	-0.75896	0.97121	2.25	-0.00006
2.25	0.15182	2.3	-0.61764	0.79704	2.3	-0.02295
2.3	0.28082	2.35	-0.49287	0.63775	2.35	-0.07833
2.35	0.40173	2.4	-0.40863	0.50540	2.4	-0.10523
2.4	0.51244	2.45	-0.35930	0.40199	2.45	-0.11308
2.45	0.61075	2.5	-0.33298	0.32408	2.5	-0.11317
2.5	0.69636	2.55	-0.32068	0.26671	2.55	-0.11078
2.55	0.76815	2.6	-0.31665	0.22532	2.601	-0.11101
2.6	0.82662	2.65	-0.31724	0.19635	2.65	-0.11333
2.65	0.87245	2.7	-0.32009	0.17725	2.7	-0.11832
2.7	0.90630	2.75	-0.32352	0.16638	2.75	-0.12609
2.75	0.92894	2.792	-0.32585	0.16297	2.79	-0.13488
2.8	0.94229	2.851	-0.32669	0.16676	2.821	-0.14400
2.82	0.94521	2.9	-0.32355	0.17794	2.84	-0.15247
2.84	0.94669	2.95	-0.31451	0.19763	2.881	-0.17016
2.86	0.94695	3.01	-0.29194	0.23212	2.9	-0.18001
2.88	0.94606	3.05	-0.26823	0.25929	2.95	-0.21168
2.9	0.94409	3.1	-0.23086	0.29164	3.01	-0.26054
2.95	0.93482	3.15	-0.19154	0.31578	3.05	-0.29691
3	0.92010	3.2	-0.15688	0.32966	3.1	-0.33978

R/Å	$2^1\Pi_g - e^1\Sigma_u^-$	$h^1\Phi_g - g^1\Delta_u$	$f^1\Pi_g - g^1\Delta_u$	$f^1\Pi_g - 2^1\Pi_u$	$d^1\Sigma_g^+ - 2^1\Pi_u$	$f^1\Pi_g - e^1\Sigma_u^-$
2.15	-0.16886	0.04152	0.34242	-0.52652	0.10717	-0.49155
2.2	-0.15001	0.03001	0.33119	-0.66723	0.06985	-0.47981
2.25	-0.13293	0.02500	0.31684	-0.76911	0.03200	-0.46549
2.3	-0.11555	0.02807	0.29805	-0.84071	0.00176	-0.44934
2.35	-0.09917	0.04156	0.27127	-0.88492	-0.02607	-0.43107

2.4	-0.08342	0.06332		0.23422	-0.90627	-0.04189	-0.41041
2.45	-0.06830	0.09021		0.18734	-0.91169	-0.05170	-0.38983
2.5	-0.05381	0.10993		0.13952	-0.90221	-0.05758	-0.36663
2.55	-0.04006	0.11873		0.10059	-0.88145	-0.06091	-0.34278
2.6	-0.02731	0.12068		0.07416	-0.84917	-0.06182	-0.32112
2.65	-0.01522	0.11397		0.05548	-0.81136	-0.06227	-0.29690
2.7	-0.00446	0.10464		0.04232	-0.76374	-0.06209	-0.27437
2.75	0.00373	0.09555		0.03502	-0.72544	-0.06134	-0.25548
2.8	0.00914	0.09451		0.03395	-0.69566	-0.05856	-0.24680
2.82	0.01281	0.08990		0.03161	-0.67498	-0.05780	-0.23789
2.84	0.01630	0.08529		0.02953	-0.65398	-0.05697	-0.22912
2.86	0.01960	0.08071		0.02769	-0.63274	-0.05608	-0.22051
2.88	0.02271	0.07619		0.02603	-0.61133	-0.05513	-0.21206
2.9	0.02965	0.06527		0.02252	-0.55753	-0.05256	-0.19174
2.95	0.03540	0.05503		0.01965	-0.50414	-0.04977	-0.17263
3	0.03997	0.04561		0.01719	-0.45208	-0.04683	-0.15483
3.05	0.04340	0.03708		0.01501	-0.40212	-0.04382	-0.13838
3.1	0.04578	0.02945		0.01303	-0.35489	-0.04081	-0.12329

Table S6. The transition dipole moment $<\Psi_{v'}|er|\Psi_{v''}> (TDM_{v',v''})$, oscillator strength f and the Einstein spontaneous emission coefficient A for the v'- v'' band of allowed electronic transitions for Si$_2$.

v''	$TDM_{0,v''}$(a.u.)	$f_{0,v''}$	$A_{0,v''}$(s^{-1})
$c^1\Sigma^+_g$ - $b^1\Pi_u$			
0	0.074248	1.28E-05	1.2386
$c^1\Sigma^+_g$ - $2^1\Pi_u$			
26	0.002725	9.32E-07	265.5132
27	0.00353	1.54E-06	424.0484
28	0.004402	2.35E-06	627.5400
29	0.005292	3.34E-06	862.4196
30	0.006143	4.43E-06	1105.1684
31	0.006853	5.42E-06	1307.4132
32	0.007372	6.17E-06	1437.5712
33	0.007616	6.47E-06	1457.4766
34	0.007558	6.27E-06	1363.5102
35	0.007193	5.58E-06	1172.6314
36	0.006553	4.55E-06	923.7964
37	0.005707	3.39E-06	664.9790
38	0.004737	2.30E-06	434.8058
39	0.003741	1.41E-06	257.2822
40	0.002801	7.75E-07	136.7852
$b^1\Pi_u$ - $f^1\Pi_g$			
2	0.04226	7.59E-05	9914.9837
3	0.068906	1.95E-04	23610.7087
4	0.096044	3.64E-04	40946.7023
5	0.118315	5.31E-04	55283.4776
6	0.131033	6.26E-04	60116.7523
7	0.13226	6.12E-04	54094.5062
8	0.122922	5.06E-04	41100.8084
9	0.105878	3.59E-04	26706.0229
10	0.084902	2.21E-04	14969.1703
11	0.063608	1.18E-04	7287.0309
12	0.044676	5.55E-05	3100.6481
$b^1\Pi_u$ - $2^1\Pi_g$			
2	0.09898	5.55E-04	128810.0705
3	0.177142	1.73E-03	379986.5199
4	0.265474	3.78E-03	784671.9145
5	0.344187	6.17E-03	1210779.2940
6	0.392453	7.79E-03	1442714.1909
7	0.398689	7.81E-03	1362214.7288
8	0.364274	6.32E-03	1038534.2360

9	0.301017	4.19E-03	646428.8001
10	0.225702	2.28E-03	330621.1606
11	0.153833	1.03E-03	139438.9758
12	0.095409	3.82E-04	48590.2802
$b^1\Pi_u - d^1\Sigma^+_g$			
0	0.45384	5.24E-03	61148.3994
1	0.12803	3.66E-04	3288.9584
$a^1\Delta_g - b^1\Pi_u$			
0	0.152937	9.05E-05	97.9263
1	0.012159	3.65E-07	0.1608
$a^1\Delta_g - 2^1\Pi_u$			
23	0.003761	9.12E-07	273.8121
24	0.004712	1.41E-06	407.6119
25	0.005666	2.00E-06	558.6963
26	0.006564	2.63E-06	710.7926
27	0.007292	3.19E-06	831.2889
28	0.007784	3.57E-06	897.3506
29	0.007965	3.67E-06	889.7909
30	0.007804	3.46E-06	808.7306
31	0.007314	2.99E-06	672.3060
32	0.006538	2.34E-06	508.4341
33	0.005567	1.67E-06	348.7647
34	0.004499	1.07E-06	215.4351
35	0.003441	6.14E-07	119.2033
36	0.00248	3.13E-07	58.5582
37	0.001676	1.40E-07	25.2928
$a^1\Delta_g - g^1\Delta_u$			
3	0.103864	8.00E-04	318561.0781
4	0.151372	1.67E-03	639726.5991
5	0.195702	2.74E-03	1010301.7219
6	0.228267	3.65E-03	1297896.7169
7	0.242848	4.06E-03	1386243.6343
8	0.238096	3.82E-03	1256648.3471
9	0.216511	3.10E-03	979387.0456
10	0.183058	2.17E-03	659461.1174
11	0.144532	1.33E-03	386943.6033
12	0.107257	7.16E-04	200447.8659
13	0.07478	3.41E-04	91612.6186
$D^3\Pi_u - C^3\Pi_g$			
1	0.019658	1.75E-05	2585.4367
2	0.039269	6.73E-05	9276.8799

3	0.061222	1.58E-04	20214.5385
4	0.079481	2.56E-04	30445.3800
5	0.089092	3.10E-04	34066.3091
6	0.088033	2.91E-04	29515.0651
7	0.077789	2.18E-04	20371.0543
8	0.062132	1.33E-04	11439.9897
9	0.045185	6.74E-05	5302.1235
10	0.030057	2.85E-05	2046.1476
$D^3\Pi_u$ - $2^3\Pi_g$			
1	0.011734	7.60E-06	1672.5606
2	0.018713	1.88E-05	3899.9834
3	0.023955	2.99E-05	5848.5011
4	0.02606	3.43E-05	6321.8399
5	0.024839	3.02E-05	5234.5181
6	0.021076	2.11E-05	3427.7326
7	0.016081	1.19E-05	1810.9604
8	0.011097	5.47E-06	780.7426
9	0.006921	2.06E-06	274.2520
10	0.003864	6.19E-07	76.9858
$D^3\Pi_u$ - $2^3\Sigma_g^-$			
48	0.001018	5.52E-08	2.8358
49	0.001497	1.16E-07	5.5526
50	0.002117	2.24E-07	10.0418
51	0.00287	3.97E-07	16.6836
52	0.003718	6.44E-07	25.2806
53	0.005811	1.52E-06	55.7566
54	0.005328	1.24E-06	42.3140
55	0.005811	1.42E-06	45.4420
56	0.005874	1.40E-06	41.9360
57	0.005418	1.15E-06	32.2486
58	0.004463	7.56E-07	19.7090
$D^3\Pi_u$ - $3^3\Pi_g$			
3	0.03844	1.02E-04	35111.5607
4	0.058289	2.29E-04	75418.1764
5	0.077994	4.01E-04	126008.9031
6	0.093825	5.67E-04	170002.3660
7	0.102813	6.65E-04	190108.0411
8	0.103647	6.60E-04	179730.6590
9	0.096783	5.61E-04	145619.3684
10	0.084095	4.13E-04	102042.1316
11	0.06822	2.65E-04	62251.1510

12	0.051825	1.49E-04	33261.1326
13	0.037006	7.41E-05	15681.0839
$D^3\Pi_u - L^3\Pi_g$			
0	0.06986	4.28E-04	238185.7579
1	0.058949	2.99E-04	160557.9738
2	0.026566	5.97E-05	30852.4175
$X^3\Sigma^-_g - D^3\Pi_u$			
0	0.193554	1.14E-04	18.9368
1	0.173771	6.56E-07	0.0000056
$X^3\Sigma^-_g - 2^3\Pi_u$			
38	0.001006	7.79E-08	8.3170
39	0.001215	1.10E-07	11.1574
40	0.00142	1.47E-07	14.0164
41	0.001604	1.82E-07	16.4348
42	0.00175	2.10E-07	17.9288
43	0.001838	2.25E-07	18.1198
44	0.001855	2.23E-07	16.8768
45	0.001793	2.02E-07	14.3964
46	0.001652	1.66E-07	11.1526
47	0.001444	1.23E-07	7.7626
48	0.001189	8.08E-08	4.7812
49	0.000911	4.60E-08	2.5486
50	0.000638	2.18E-08	1.1344
51	0.000395	8.11E-09	0.3944
52	0.000201	2.02E-09	0.0918
53	0.000062	1.85E-10	0.0078
$X^3\Sigma^-_g - H^3\Sigma^-_u$			
6	0.117423	8.85E-04	263884.6959
7	0.165057	1.71E-03	487339.2212
8	0.213514	2.80E-03	761434.5672
9	0.256353	3.94E-03	1023775.9568
10	0.287824	4.85E-03	1202428.2081
11	0.303354	5.26E-03	1243141.0582
12	0.300499	5.04E-03	1134050.3879
13	0.280603	4.29E-03	918133.1197
14	0.248277	3.27E-03	666511.4629
15	0.208621	2.25E-03	435860.1793
16	0.166095	1.39E-03	255564.1232
17	0.125289	7.71E-04	134307.6450
18	0.090244	3.89E-04	64251.5424
$A^3\Sigma^+_u - 2^3\Pi_g$			

0	0.047406	4.08E-05	243.6206
1	0.065818	7.08E-05	341.5304
2	0.066342	6.40E-05	244.6444
3	0.054762	3.84E-05	113.3726
4	0.037358	1.55E-05	34.3472
5	0.019584	3.62E-06	5.8230
6	0.004376	1.50E-07	0.1664
$A^3\Sigma^+_u$ - $3^3\Pi_g$			
0	0.117434	7.19E-04	35254.2952
1	0.114882	6.64E-04	30307.2758
2	0.086699	3.64E-04	15475.6484
3	0.056562	1.49E-04	5897.6264
4	0.032356	4.71E-05	1726.2372
$A^3\Sigma^+_u$ - $L^3\Pi_g$			
3	0.007066	3.73E-06	376.1858
4	0.007066	3.65E-06	351.0086
5	0.018733	2.50E-05	2303.4220
6	0.02736	5.22E-05	4589.9166
7	0.018733	2.39E-05	2013.9850
8	0.02736	5.00E-05	4028.6116
9	0.046746	1.43E-04	11054.3830
10	0.038567	9.53E-05	7080.3906
11	0.023897	3.59E-05	2556.6654
$B^3\Delta_u$ - $2^3\Pi_g$			
0	0.049794	2.52E-05	188.2762
1	0.070571	4.58E-05	280.5640
2	0.075901	4.75E-05	233.8650
3	0.071191	3.71E-05	143.2513
4	0.061216	2.39E-05	70.6813
5	0.050223	1.38E-05	30.0527
6	0.03925	7.06E-06	10.7190
7	0.029936	3.31E-06	3.2772
8	0.022292	1.40E-06	0.8077
$B^3\Delta_u$ - $E^3\Phi_g$			
0	0.068175	6.16E-05	780.8197
1	0.087037	9.30E-05	1014.7552
2	0.084054	8.01E-05	742.9175
3	0.070714	5.20E-05	405.7512
4	0.054498	2.81E-05	182.3589
5	0.040067	1.37E-05	72.8692
6	0.028036	6.02E-06	25.5701

7	0.019151	2.49E-06	8.2583
$B^3\Delta_u - 3^3\Pi_g$			
0	0.077972	1.65E-04	8778.5241
1	0.078405	1.61E-04	7964.3126
2	0.062897	9.98E-05	4586.0071
3	0.045692	5.07E-05	2160.1410
4	0.031305	2.29E-05	902.7368
5	0.020941	9.85E-06	358.6841
$B^3\Delta_u - L^3\Pi_g$			
5	0.008972	2.93E-06	281.5238
6	0.011744	4.90E-06	447.5412
7	0.014603	7.39E-06	641.5841
8	0.01736	1.02E-05	839.6340
9	0.019895	1.30E-05	1020.5560
10	0.022066	1.56E-05	1160.6104
11	0.023805	1.77E-05	1247.7139
12	0.02502	1.90E-05	1271.9037
13	0.02575	1.96E-05	1242.1600
14	0.025938	1.94E-05	1160.9821
15	0.025698	1.85E-05	1048.8665
16	0.025015	1.70E-05	913.8931
17	0.024004	1.53E-05	773.1633
18	0.022716	1.33E-05	635.6808
19	0.021217	1.13E-05	508.6970
20	0.019598	9.33E-06	397.8220
21	0.017898	7.56E-06	303.9315
22	0.01736	6.90E-06	261.7769
23	0.014494	4.67E-06	166.9740
$X^3\Sigma_g^- - K^3\Sigma_u^-$			
0	0.224095	4.68E-03	2935611.9831
1	0.201324	3.72E-03	2258109.3621
2	0.201324	3.66E-03	2151329.8317
3	0.117821	1.23E-03	701553.6955
4	0.062387	3.40E-04	187189.6189
5	0.031644	8.60E-05	45809.4903
$X^3\Sigma_g^- - 3^3\Sigma_u^-$			
23	0.022172	3.95E-05	18486.9599
24	0.031058	7.64E-05	34640.2028
25	0.041806	1.36E-04	59919.4127
26	0.054205	2.26E-04	96141.6147
27	0.067389	3.43E-04	141786.8630

28	0.080166	4.78E-04	191400.8938
29	0.091212	6.09E-04	236296.3533
30	0.098844	7.04E-04	264559.7785
31	0.101884	7.36E-04	267916.8544
32	0.099583	6.92E-04	243897.6217
33	0.092053	5.82E-04	198543.8070
34	0.080313	4.36E-04	143938.7783
35	0.065994	2.90E-04	92543.4567
36	0.051083	1.71E-04	52785.0866
37	0.037297	8.95E-05	26781.6251
$2\,{}^1\Pi_u$-$f\,{}^1\Pi_g$			
6	0.026702	2.8018E-05	3127.5614
7	0.051184	1.0101E-04	10853.5623
8	0.085440	2.7618E-04	28574.2548
9	0.124202	5.7308E-04	57171.8115
10	0.152212	8.4546E-04	81384.9845
11	0.154582	8.5721E-04	79739.3344
12	0.122512	5.2958E-04	47657.4509
13	0.068717	1.6400E-04	14299.5810
14	0.019905	1.3556E-05	1146.9979
$g\,{}^1\Delta_u$-$f\,{}^1\Pi_g$			
0	0.047487	6.5169E-05	3934.4240
1	0.039037	4.2653E-05	2415.4030
2	0.020392	1.1269E-05	598.3111
3	0.007458	1.4592E-06	72.6164
4	0.002154	1.1783E-07	5.4955
$f\,{}^1\Pi_g$-$e\,{}^1\Sigma_u^-$			
0	0.198450	1.2155E-03	20926.6941
1	0.200349	1.1614E-03	17568.9243
2	0.165421	7.3957E-04	9762.6760
3	0.124134	3.8733E-04	4422.5378
4	0.087789	1.7940E-04	1756.7938
5	0.060663	7.9000E-05	657.9402
6	0.040506	3.2251E-05	225.1853
7	0.026593	1.2652E-05	73.1731
8	0.017309	4.8330E-06	22.7282
$2\,{}^1\Pi_g$-$e\,{}^1\Sigma_u^-$			
0	0.026126	4.0385E-05	2555.0010
1	0.025217	3.6396E-05	2154.6743
2	0.015711	1.3658E-05	755.5849
3	0.008651	3.9996E-06	206.4081

4	0.004552	1.0688E-06	51.3900
5	0.002445	2.9752E-07	13.3183
6	0.001246	7.4477E-08	3.0957
7	0.000599	1.6565E-08	0.6387
$2^3\Pi_u$-$C^3\Pi_g$			
18	0.013565	3.9787E-06	134.4534
19	0.021718	9.8337E-06	308.9747
20	0.032375	2.1067E-05	615.2353
21	0.044671	3.8665E-05	1049.3693
22	0.056313	5.9236E-05	1494.0783
23	0.063813	7.3339E-05	1719.6028
24	0.063350	6.9706E-05	1520.1596
25	0.052692	4.6528E-05	944.5174
26	0.033721	1.8395E-05	347.9973
27	0.013197	2.7220E-06	48.0556
$H^3\Sigma^-_u$ -$C^3\Pi_g$			
0	0.008897	3.9101E-06	172.4014
1	0.020233	1.9324E-05	778.1092
2	0.030662	4.2344E-05	1552.3558
3	0.036006	5.5619E-05	1849.9816
4	0.034870	4.9602E-05	1491.6505
5	0.028521	3.1492E-05	852.9413
6	0.020117	1.4835E-05	360.2942
7	0.012320	5.2583E-06	114.0305
8	0.006395	1.3351E-06	25.7220
9	0.002669	2.1859E-07	3.7213
$K^3\Sigma^-_u$ -$C^3\Pi_g$			
0	0.173818	2.7102E-03	394116.2656
1	0.065048	3.7029E-04	51249.2029
$3^3\Sigma^-_u$ -$C^3\Pi_g$			
9	0.002053	4.5599E-07	96.5386
10	0.005111	2.7771E-06	567.4072
11	0.009646	9.7179E-06	1916.0287
12	0.015035	2.3196E-05	4413.5554
13	0.019961	4.0167E-05	7376.9636
14	0.023473	5.4572E-05	9674.8522
15	0.025536	6.3464E-05	10863.5846
16	0.025759	6.3462E-05	10491.1585
17	0.023212	5.0649E-05	8088.7704
18	0.017192	2.7316E-05	4215.8019
19	0.009920	8.9416E-06	1334.2232

20	0.004716	1.9878E-06	286.9158
21	0.002124	3.9662E-07	55.4085
$2^3\Sigma_g^-$ -$2^3\Pi_u$			
0	0.019894	1.1990E-06	0.1989
1	0.016144	5.3634E-07	0.0410
2	0.010024	1.1065E-07	0.0024
3	0.005377	4.6535E-09	0.0000
$L^3\Pi_g$-$2^3\Pi_u$			
0	0.027541	8.0411E-06	65.3281
1	0.030537	8.8545E-06	57.7082
2	0.022565	4.2860E-06	21.9531
3	0.012893	1.2247E-06	4.8057
4	0.005792	2.1278E-07	0.6187
$2^3\Pi_u$-$2^3\Pi_g$			
17	0.014462	2.8477E-06	38.1639
18	0.014462	2.6834E-06	31.9326
19	0.033226	1.3309E-05	139.8347
20	0.046363	2.4274E-05	223.7599
21	0.061160	3.9425E-05	316.5982
22	0.076262	5.6987E-05	395.5062
23	0.089718	7.2991E-05	433.8645
24	0.099379	8.2455E-05	415.4544
25	0.103348	8.1611E-05	344.4235
26	0.100456	7.0080E-05	244.3027
27	0.090809	5.1620E-05	146.2132
28	0.075820	3.2117E-05	72.4679
29	0.058062	1.6608E-05	29.1349
30	0.040553	7.0355E-06	9.3081
31	0.025790	2.4229E-06	2.3239
32	0.014958	6.7573E-07	0.4455
33	0.007774	1.4569E-07	0.0612
$H^3\Sigma_u^-$ -$2^3\Pi_g$			
0	0.027582	2.2439E-05	352.8047
1	0.066488	1.2141E-04	1654.7134
2	0.098366	2.4634E-04	2885.4100
3	0.106464	2.6620E-04	2653.3939
4	0.093843	1.8974E-04	1591.7650
5	0.070736	9.8223E-05	684.0333
6	0.044169	3.4620E-05	197.0133
7	0.021872	7.6026E-06	34.7011
8	0.009609	1.2987E-06	4.6434

$K^3\Sigma^-_u$ -$2^3\Pi_g$			
0	0.254857	4.5340E-03	399267.1813
1	0.104355	7.3804E-04	61261.0373
2	0.021852	3.1406E-05	2455.0043
$3^3\Sigma^-_u$ -$2^3\Pi_g$			
8	0.008419	6.4933E-06	984.7847
9	0.015047	2.0336E-05	2964.7860
10	0.024339	5.2162E-05	7308.9976
11	0.035976	1.1171E-04	15040.6554
12	0.048263	1.9707E-04	25491.5018
13	0.058515	2.8391E-04	35272.0981
14	0.063947	3.3226E-04	39640.4363
15	0.062243	3.0843E-04	35327.3389
16	0.053567	2.2380E-04	24604.0737
17	0.040060	1.2261E-04	12934.1271
18	0.025623	4.9130E-05	4971.7972
19	0.013708	1.3771E-05	1336.4449
20	0.006074	2.6473E-06	246.3232
$2^1\Pi_u$-$d^1\Sigma^+_g$			
22	0.001766	2.7422E-07	38.3455
23	0.002912	7.2646E-07	96.3690
24	0.004570	1.7435E-06	219.4950
25	0.006759	3.7150E-06	443.9989
26	0.009406	7.0114E-06	795.8802
27	0.012205	1.1510E-05	1241.7094
28	0.014635	1.6138E-05	1655.6665
29	0.016041	1.8915E-05	1847.1885
30	0.015819	1.7958E-05	1671.0288
31	0.013739	1.3231E-05	1174.5132
32	0.010162	7.0743E-06	599.9486
33	0.006049	2.4523E-06	198.9970
34	0.002598	4.4298E-07	34.4580
35	0.000564	2.0454E-08	1.5283
$3^3\Sigma^-_u$ - $2^3\Sigma^-_g$			
2	0.018148	7.3517E-06	264.7980
3	0.032184	2.2738E-05	792.1231
4	0.049277	5.2420E-05	1765.8552
5	0.067537	9.6824E-05	3153.7507
6	0.084820	1.5017E-04	4729.3368
7	0.099053	2.0139E-04	6132.9405
8	0.108760	2.3877E-04	7032.6138

9	0.112411	2.5088E-04	7148.7606
10	0.112411	2.4682E-04	6806.6738
11	0.107047	2.2025E-04	5881.8158
12	0.098223	1.8253E-04	4723.0931
13	0.087280	1.4192E-04	3560.6908
14	0.075495	1.0460E-04	2546.8484
15	0.063821	7.3681E-05	1742.8190
16	0.052916	4.9955E-05	1149.3231
17	0.043203	3.2865E-05	736.4854
18	0.034849	2.1120E-05	461.6745
19	0.027862	1.3343E-05	284.9377
20	0.022000	8.2291E-06	171.9586
21	0.017492	5.1509E-06	105.5121
22	0.013866	3.2071E-06	64.5059
23	0.011216	2.0811E-06	41.1647
24	0.009170	1.3808E-06	26.9114
$2\,^3\Sigma_g^- - H\,^3\Sigma_u^-$			
11	0.029789	6.6368E-06	26.8345
12	0.048652	1.6093E-05	53.7719
13	0.074266	3.3820E-05	91.9232
14	0.105427	6.0891E-05	132.0989
15	0.139307	9.3931E-05	159.0700
16	0.171580	1.2416E-04	159.6317
17	0.196491	1.3939E-04	131.3446
18	0.209570	1.3266E-04	87.4864
19	0.208267	1.0617E-04	45.9842
20	0.191827	6.9647E-05	18.0349
21	0.162118	3.5634E-05	4.7352
22	0.123535	1.2776E-05	0.6472
23	0.083051	2.3198E-06	0.0190
$3\,^3\Pi_g - 2\,^3\Sigma_u^+$			
0	0.109194	3.1710E-04	4053.0709
1	0.038535	3.5565E-05	368.6742
2	0.006390	8.7699E-07	7.3101
3	0.001134	2.4614E-08	0.1631
$L\,^3\Pi_g - 2\,^3\Sigma_u^+$			
0	0.055816	1.7002E-04	9150.5045
1	0.070737	2.5984E-04	12662.2882
2	0.074138	2.7182E-04	12014.3815
3	0.071654	2.4196E-04	9710.8548
4	0.066004	1.9574E-04	7140.4853

5	0.059103	1.4968E-04	4966.6764
6	0.051566	1.0872E-04	3284.9607
7	0.044381	7.6899E-05	2118.1059
8	0.037527	5.2553E-05	1322.5782
9	0.031843	3.6207E-05	834.2295
10	0.026601	2.4203E-05	511.6876
11	0.022370	1.6417E-05	319.3238
12	0.018664	1.0981E-05	197.1704
13	0.015624	7.4063E-06	123.1938
14	0.013135	5.0492E-06	78.1449
15	0.011024	3.4390E-06	49.7661
$K^3\Sigma^-_u$ - $L^3\Pi_g$			
0	0.023563	4.3820E-06	4.9327
1	0.037559	6.4157E-06	2.3982
2	0.036136	1.7733E-06	0.0591
$g^1\Delta_u$-$h^1\Phi_g$			
0	0.053375	4.2016E-05	660.6078
1	0.070119	6.7369E-05	914.2721
2	0.056652	4.0649E-05	471.3771
3	0.034782	1.4084E-05	137.9761
4	0.017114	3.1131E-06	25.4233
$1^5\Pi_g - 1^5\Pi_u$			
30	0.111069	1.6167E-04	2007.2782
31	0.125013	1.9364E-04	2148.8833
32	0.137266	2.2029E-04	2176.4707
33	0.146822	2.3730E-04	2078.7017
34	0.152906	2.4180E-04	1869.5396
35	0.154914	2.3261E-04	1579.7225
36	0.152413	2.1047E-04	1248.9279
37	0.145445	1.7866E-04	921.1275
38	0.134437	1.4184E-04	631.5019
39	0.120077	1.0480E-04	400.1972