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Energy Levels and Radiative Rates for Transitions in F-like Sc XIII and Ne-like Sc XII and Y XXX

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Abstract: Energy levels, radiative rates and lifetimes are reported for F-like Sc XIII and Ne-like Sc XII and Y XXX for which the general-purpose relativistic atomic structure package (GRASP) has been adopted. For all three ions, limited data exist in the literature but comparisons have been made wherever possible to assess the accuracy of the calculations. In the present work, the lowest 102, 125 and 139 levels have been considered for the respective ions. Additionally, calculations have also been performed with the flexible atomic code (FAC) to (particularly) confirm the accuracy of energy levels.

Keywords: rare earth elements; energy levels; radiative rates; lifetimes; F-like and Ne-like ions

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1. Introduction

Atomic data for several parameters, including energy levels and radiative rates, are required for the diagnostics and modelling of plasmas. Often, the required data are not available experimentally and therefore it becomes necessary to obtain theoretical results. Consequently, a vast amount of theoretical data are available in the literature for a (very) wide range of ions. However, comparatively neglected are the rare earth elements (Sc, Y and those with $57 \leq Z \leq 71$), although work on their ions is gradually picking momentum. In this paper, we report atomic data for F-like Sc XIII and Ne-like Sc XII and Y XXX.

The importance of Sc ions was realised early by Pryce [1], who speculated that their emission lines may be observed in the visible or near-visible regions of the coronal plasma. However, to the best of our knowledge, no lines of Sc XII or Sc XIII have been observed so far in the astrophysical plasmas. This may also be confirmed by the CHIANTI (http://www.chiantidatabase.org/) database, which stores data for all ions of astrophysical importance, but none for the Sc ions. Nevertheless, several lines of Sc XIII have been measured by Jupén et al. [2] in the laser-produced plasmas. Similarly, energy levels and radiative rates (A-values) have been determined for several ions of the F sequence of which the work by Jönsson et al. [3] is not only the latest, but also the most accurate because differences with the measurements are minimal for the energy levels. Unfortunately, they calculated data only for the lowest three levels of the $2s^22p^5$ and $2s2p^6$ configurations, which are not sufficient for modelling of plasmas because the data are required for a wider range of levels. Therefore, in this work, we cover a much wider range of levels, discussed in Section 2. We also note here that similar data for F-like Y XXXI are not considered here because results have already been reported in a separate paper [4].

Ne-like ions are of interest for the studies of astrophysical, lasing and fusion plasmas, and therefore many workers, such as [5–10], have reported data for a wide range of ions. However, for brevity, many of them have not reported data for Sc XII, although Hibbert et al. [9] have listed lifetimes (τ) for the lowest 27 levels of the $2s^22p^6$ and $2s^22p^53\ell$ configurations. The only other results available for comparisons are those of Cogordan and Lunell [5] and Jönsson et al. [10], but are limited to the lowest 27 levels of the $2s^22p^6$ and $2s^22p^53\ell$ configurations. Therefore, there is a clear need to expand the range of levels for this ion. Similarly, limited results are available in the literature for Y XXX, mainly by [5–8], whereas Nilsen and Scofield [11] and Silwal et al. [12] have measured wavelengths for a few transitions of this ion, which is of particular interest for the diagnostics of tokamak fusion plasmas, as it is one of the impurity elements. Therefore, our aim is to report a complete set of data for energies and lifetimes for a larger number of levels for all three above named ions and A-values for all transitions among their levels, not only for the dominant allowed electric dipole (E1) type, but also for electric quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2), which are not only required for complete and reliable plasma models, but are also useful for more accurate determination of lifetimes.

2. Energy Levels

As in our earlier work on several F-like [4,13] and Ne-like [14,15] ions, we adopt the fully relativistic GRASP (general-purpose relativistic atomic structure package) code of Grant et al. [16] to determine the atomic structure, and subsequently to calculate energy levels and A-values. However, this earlier version has been significantly revised by Dr. P.H. Norrington (one of the authors), and is currently hosted at the website: http://amdpp.phys.strath.ac.uk/UK_APAP/codes.html. Similarly, the option of extended average level (EAL), in which a weighted (proportional to $2j$+1) trace of the Hamiltonian matrix is minimized, is used. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. This also provides comparable results with other options such as average level (AL).

Since both Sc and Y are moderately heavy elements, both relativistic effects and configuration interaction (CI) are important for the determination of atomic structures. Our adopted version of the GRASP code is fully relativistic, as are the other ones, such as GRASP2K [17], but it cannot handle the inclusion of an extensive CI, or a very large number of configuration state functions (CSF). Therefore, we have also performed calculations with the *Flexible Atomic Code* (FAC) of Gu [18], hosted at the website https://www-amdis.iaea.org/FAC/. This is also a fully relativistic code and provides a variety of atomic parameters. Not only the code yields data, which, in most instances, are comparable to those generated with GRASP, but the inclusion of a very large CI is also possible with ease and efficiency. Therefore, these parallel calculations serve two purposes, i.e., firstly, the accuracy of the determined energy levels can be assessed, and this is necessary because similar results for a majority of levels are not available with which to compare, as already stated in Section 1, and secondly, the effect of larger CI (if any) can be quantified.

2.1. Sc XIII

With GRASP, we have performed a series of calculations with increasing CI, but mention here only three, namely (i) GRASP1, which includes 113 levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43\ell$, $2s2p^53\ell$, and $2p^63\ell$ (11) configurations; (ii) GRASP2, which includes a further eight of $2s^22p^44\ell$ and $2s2p^54\ell$, giving rise to additional 159 levels; and finally (iii) GRASP3, which includes 501 levels in total from 38 configurations, the additional ones being $2p^64\ell$, $2s^22p^45\ell$, $2s2p^55\ell$, and $2p^65\ell$. However, for brevity, we will discuss results from only our final calculations, but the effect of additional CI will be discussed with those from FAC.

As with GRASP, with FAC too we have performed a series of calculations, but focus on only three, i.e., (i) FAC1, which includes 113 levels as in GRASP1, (ii) FAC2, which includes 501 levels as in GRASP3, and finally (iii) FAC3, which includes in total 38 089 levels arising from all possible combinations of the (2*5) 3*2, 4*2, 5*2, 3*1 4*1, 3*1 5*1, and 4*1 5*1 configurations, plus those of FAC2. Although calculations have also been performed with even larger CI, these are not discussed here because the calculated energy levels show no appreciable differences, either in magnitude or orderings, i.e., the results have fully converged in FAC3. For brevity, for FAC calculations, we have used a short notation here (and elsewhere in the text) for describing configurations. As an example, 3*2 means $3\ell3\ell'$ resulting in 3s3p, 3s3d, 3p3d, $3s^2$, $3p^2$, and $3d^2$.

Our calculated energies for the *lowest* 102 levels of Sc XIII are listed in Table 1. These levels mostly belong to the $2s^22p^5$, $2s2p^6$, $2s^22p^43\ell$, and $2s2p^53\ell$ configurations, and beyond these from others intermix, such as $2s^22p^44\ell$. However, energies for higher levels can be obtained from the author on request. Our energies calculated with GRASP, *without* and *with* the inclusion of Breit and QED (quantum electro-dynamic) effects, are listed in the table, along with all three calculations with the FAC, mentioned above. In addition, the experimental energies, compiled by the NIST (National Institute for Standards and Technology) team and available at the website http://www.nist.gov/pml/data/asd.cfm, are listed here along with the theoretical results of Jupén et al. [2], obtained from the Hartree–Fock Relativistic (HFR) code of Cowan—see [19]. However, these theoretical results have been adjusted with *least square fitting* with the available measurements for a few levels, and that is the reason that there are no appreciable differences for the levels in common with the NIST. We also note that, for two levels (40/41), the NIST and HFR energies are non differentiable, but not in any of our calculations with both codes.

Table 1. Energies (in Ryd) and lifetimes (τ, s) for the lowest 102 levels of Sc XIII. $a \pm b \equiv a \times 10^{\pm b}$.

Index	Configuration	Level	NIST	HFR	GRASP1	GRASP2	FAC1	FAC2	FAC3	τ (GRASP2)
1	$2s^22p^5$	$^2P^o_{3/2}$	0.000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	....
2	$2s^22p^5$	$^2P^o_{1/2}$	0.345	0.3458	0.3543	0.3430	0.3426	0.3424	0.3425	1.045-03
3	$2s2p^6$	$^2S_{1/2}$	6.959	6.9588	7.1071	7.0978	7.1152	7.1021	7.0877	1.363-11
4	$2s^22p^43s$	$^4P_{5/2}$	32.016	32.0155	31.9299	31.9067	31.9416	31.9404	31.7915	9.843-11
5	$2s^22p^43s$	$^4P_{3/2}$	32.173	32.1703	32.0898	32.0666	32.1064	32.1073	31.9452	3.494-12
6	$2s^22p^43s$	$^4P_{1/2}$	32.324	32.3235	32.2361	32.2104	32.2440	32.2429	32.0925	6.617-11
7	$2s^22p^43s$	$^2P_{3/2}$	32.394	32.3937	32.3158	32.2906	32.3375	32.3419	32.1612	1.623-12
8	$2s^22p^43s$	$^2P_{1/2}$	32.570	32.5696	32.4940	32.4684	32.5216	32.5282	32.3353	1.093-12
9	$2s^22p^43s$	$^2D_{5/2}$	32.983	32.9833	32.9299	32.8984	32.9169	32.9188	32.7710	2.825-12
10	$2s^22p^43s$	$^2D_{3/2}$	32.995	32.9951	32.9402	32.9088	32.9285	32.9308	32.7803	2.613-12
11	$2s^22p^43p$	$^4P^o_{5/2}$		33.5910	33.5112	33.4860	33.5231	33.5164	33.3813	4.776-10
12	$2s^22p^43p$	$^4P^o_{3/2}$		33.6070	33.5246	33.5032	33.5404	33.5341	33.3978	4.386-10
13	$2s^22p^43p$	$^4P^o_{1/2}$		33.7247	33.6439	33.6209	33.6564	33.6488	33.5135	4.412-10
14	$2s^22p^43p$	$^4D^o_{7/2}$		33.7869	33.7148	33.6891	33.7260	33.7283	33.5782	2.996-10
15	$2s^22p^4(^3P)3p$	$^2D^o_{5/2}$		33.8297	33.7568	33.7331	33.7528	33.7554	33.6173	3.445-10
16	$2s^22p^43s$	$^2S_{1/2}$	33.885	33.8851	33.7722	33.7480	33.7750	33.7791	33.6554	2.766-12
17	$2s^22p^4(^3P)3p$	$^2P^o_{1/2}$		33.9692	33.9064	33.8823	33.9155	33.9094	33.7678	2.856-10
18	$2s^22p^43p$	$^4D^o_{3/2}$		33.9882	33.9151	33.8892	33.9264	33.9289	33.7729	3.208-10
19	$2s^22p^43p$	$^4D^o_{1/2}$		34.0260	33.9515	33.9265	33.9635	33.9658	33.8135	2.813-10
20	$2s^22p^43p$	$^4D^o_{5/2}$		34.0802	34.0104	33.9827	34.0211	34.0248	33.8624	3.175-10
21	$2s^22p^4(^3P)3p$	$^2P^o_{3/2}$		34.1222	34.0295	34.0001	34.0359	34.0291	33.8819	2.730-10
22	$2s^22p^43p$	$^4S^o_{3/2}$		34.1913	34.1203	34.0949	34.1350	34.1412	33.9804	1.730-10
23	$2s^22p^4(^3P)3p$	$^2S^o_{1/2}$		34.2408	34.1738	34.1455	34.1823	34.1861	34.0219	3.267-10
24	$2s^22p^4(^3P)3p$	$^2D^o_{3/2}$		34.2327	34.1795	34.1505	34.1919	34.1968	34.0268	2.310-10
25	$2s^22p^43p$	$^2F^o_{5/2}$		34.5951	34.5491	34.5172	34.5357	34.5381	34.3973	3.788-10
26	$2s^22p^43p$	$^2F^o_{7/2}$		34.6571	34.6149	34.5803	34.5979	34.5998	34.4607	3.335-10
27	$2s^22p^4(^1D)3p$	$^2D^o_{3/2}$		34.8134	34.7669	34.7375	34.7570	34.7635	34.6168	2.215-10
28	$2s^22p^4(^1D)3p$	$^2D^o_{5/2}$		34.8524	34.8089	34.7765	34.7965	34.8037	34.6550	2.420-10
29	$2s^22p^4(^1D)3p$	$^2P^o_{3/2}$		35.3175	35.2384	35.2135	35.2915	35.2895	35.0662	3.438-11
30	$2s^22p^4(^1D)3p$	$^2P^o_{1/2}$		35.3499	35.2733	35.2479	35.3197	35.2996	35.1242	3.100-11
31	$2s^22p^4(^1S)3p$	$^2P^o_{3/2}$		35.6572	35.5598	35.5353	35.5557	35.5546	35.4494	1.052-10
32	$2s^22p^4(^1S)3p$	$^2P^o_{1/2}$		35.7942	35.6876	35.6585	35.7274	35.7096	35.5420	1.080-10
33	$2s^22p^43d$	$^4D_{7/2}$		35.7683	35.6967	35.6671	35.7200	35.7015	35.5418	1.979-10
34	$2s^22p^43d$	$^4D_{5/2}$		35.7785	35.7053	35.6778	35.7450	35.7267	35.5494	1.877-10
35	$2s^22p^43d$	$^4D_{3/2}$		35.8200	35.7383	35.7131	35.7605	35.7436	35.5824	7.254-11
36	$2s^22p^43d$	$^4D_{1/2}$		35.8654	35.7854	35.7602	35.8086	35.7919	35.6295	6.519-11
37	$2s^22p^43d$	$^4F_{9/2}$		35.9488	35.8847	35.8552	35.8991	35.8891	35.7268	1.705-10
38	$2s^22p^43d$	$^4F_{7/2}$		36.0225	35.9661	35.9375	35.9733	35.9668	35.7922	1.598-10
39	$2s^22p^43d$	$^4P_{1/2}$	36.102	36.1017	36.0325	36.0065	36.0384	36.0374	35.8618	3.624-12
40	$2s^22p^43d$	$^4F_{5/2}$	36.162	36.1618	36.1014	36.0715	36.1102	36.1035	35.9298	2.505-12
41	$2s^22p^43d$	$^4P_{3/2}$	36.162	36.1618	36.1030	36.0757	36.1108	36.1083	35.9327	2.022-12
42	$2s^22p^4(^3P)3d$	$^2P_{1/2}$	36.215	36.2147	36.1592	36.1328	36.1694	36.1614	35.9864	2.918-12
43	$2s^22p^43d$	$^4F_{3/2}$		36.2171	36.1703	36.1415	36.1833	36.1737	36.0088	1.689-11

Table 1. *Cont.*

Index	Configuration	Level	NIST	HFR	GRASP1	GRASP2	FAC1	FAC2	FAC3	τ (GRASP2)
44	$2s^22p^4(^3P)3d$	$^2F_{7/2}$		36.2271	36.1716	36.1404	36.1762	36.1690	35.9923	1.708-10
45	$2s^22p^43d$	$^4P_{5/2}$	36.257	36.2575	36.1973	36.1672	36.2024	36.1985	36.0251	3.312-12
46	$2s^22p^4(^3P)3d$	$^2D_{3/2}$	36.307	36.3067	36.2530	36.2252	36.2604	36.2531	36.0767	7.388-13
47	$2s^22p^4(^3P)3d$	$^2F_{5/2}$	36.336	36.3359	36.2848	36.2537	36.2843	36.2816	36.0964	4.289-12
48	$2s^22p^4(^3P)3d$	$^2P_{3/2}$	36.453	36.4534	36.4051	36.3721	36.4022	36.3954	36.2186	1.771-12
49	$2s^22p^4(^3P)3d$	$^2D_{5/2}$	36.494	36.5236	36.4578	36.4230	36.4572	36.4527	36.2662	4.378-13
50	$2s^22p^43d$	$^2G_{7/2}$		36.7662	36.7310	36.6935	36.7185	36.7056	36.5569	1.725-10
51	$2s^22p^43d$	$^2G_{9/2}$		36.7702	36.7362	36.6980	36.7210	36.7076	36.5605	1.855-10
52	$2s^22p^4(^1D)3d$	$^2S_{1/2}$	36.945	36.9446	36.9226	36.8871	36.8926	36.8953	36.7196	1.683-13
53	$2s^22p^4(^1D)3d$	$^2F_{5/2}$	36.971	36.9710	36.9441	36.9105	36.9207	36.9199	36.7583	3.243-12
54	$2s^22p^4(^1D)3d$	$^2F_{7/2}$		37.0086	36.9805	36.9442	36.9522	36.9526	36.7894	1.494-10
55	$2s^22p^4(^1D)3d$	$^2P_{3/2}$	37.103	37.1041	37.0808	37.0477	37.0676	37.0699	36.8950	1.329-13
56	$2s^22p^4(^1D)3d$	$^2D_{5/2}$	37.104	37.1041	37.1013	37.0663	37.0875	37.0874	36.8952	1.644-13
57	$2s^22p^4(^1D)3d$	$^2D_{3/2}$	37.219	37.1889	37.2125	37.1749	37.1913	37.1936	36.9972	1.723-13
58	$2s^22p^4(^1D)3d$	$^2P_{1/2}$		37.2186	37.2138	37.1737	37.1914	37.1949	37.0132	1.250-13
59	$2s^22p^4(^1S)3d$	$^2D_{5/2}$	37.817	37.8167	37.7296	37.7007	37.6980	37.6961	37.5840	1.283-12
60	$2s^22p^4(^1S)3d$	$^2D_{3/2}$	37.873	37.8732	37.7955	37.7637	37.7723	37.7703	37.6458	3.332-13
61	$2s2p^53s$	$^4P^o_{5/2}$			38.2026	38.1736	38.2253	38.2262	38.1003	2.172-11
62	$2s2p^53s$	$^4P^o_{3/2}$			38.3683	38.3358	38.3890	38.3892	38.2588	1.090-11
63	$2s2p^53s$	$^4P^o_{1/2}$			38.5119	38.4763	38.5271	38.5275	38.3978	1.457-11
64	$2s2p^5(^3P)3s$	$^2P^o_{3/2}$	38.657		38.7074	38.6767	38.7624	38.7552	38.5795	2.206-12
65	$2s2p^5(^3P)3s$	$^2P^o_{1/2}$	38.858		38.9127	38.8779	38.9622	38.9548	38.7779	1.786-12
66	$2s2p^53p$	$^4S_{3/2}$			39.6759	39.6458	39.6939	39.6906	39.5885	2.118-11
67	$2s2p^53p$	$^4D_{7/2}$			39.9070	39.8754	39.9253	39.9294	39.8137	2.538-11
68	$2s2p^53p$	$^4D_{5/2}$			39.9142	39.8845	39.9395	39.9432	39.8207	6.173-12
69	$2s2p^53p$	$^4D_{3/2}$			40.0059	39.9752	40.0297	40.0333	39.9103	5.149-12
70	$2s2p^5(^3P)3p$	$^2D_{5/2}$			40.0974	40.0672	40.1225	40.1258	39.9996	1.897-12
71	$2s2p^53p$	$^4D_{1/2}$			40.1030	40.0700	40.1348	40.1367	40.0040	1.119-11
72	$2s2p^5(^3P)3p$	$^2P_{3/2}$			40.2049	40.1709	40.2330	40.2379	40.1008	1.138-12
73	$2s2p^53p$	$^4P_{5/2}$			40.2454	40.2083	40.2694	40.2718	40.1391	2.380-12
74	$2s2p^53p$	$^4P_{1/2}$			40.2683	40.2337	40.2965	40.2950	40.1644	8.976-12
75	$2s2p^53p$	$^4P_{3/2}$			40.2727	40.2375	40.3026	40.3034	40.1676	2.442-12
76	$2s2p^5(^3P)3p$	$^2P_{1/2}$			40.3322	40.2980	40.3619	40.3654	40.2250	8.998-13
77	$2s2p^5(^3P)3p$	$^2D_{3/2}$			40.4258	40.3874	40.4508	40.4558	40.3139	1.344-12
78	$2s2p^5(^1P)3s$	$^2P^o_{3/2}$			40.6851	40.6536	40.6805	40.6761	40.5309	2.445-12
79	$2s2p^5(^1P)3s$	$^2P^o_{1/2}$			40.7039	40.6724	40.7017	40.6969	40.5482	3.133-12
80	$2s2p^5(^3P)3p$	$^2S_{1/2}$			40.7756	40.7424	40.8127	40.7916	40.6547	6.595-13
81	$2s2p^53d$	$^4P^o_{1/2}$			41.8397	41.8097	41.8679	41.8520	41.7237	2.127-11
82	$2s2p^53d$	$^4P^o_{3/2}$			41.8813	41.8485	41.9081	41.8915	41.7630	1.966-11
83	$2s2p^53d$	$^4F^o_{9/2}$			41.9310	41.8952	41.9715	41.9390	41.8241	3.837-11
84	$2s2p^53d$	$^4P^o_{5/2}$			41.9563	41.9210	41.9821	41.9639	41.8356	2.265-11
85	$2s2p^53d$	$^4F^o_{7/2}$			41.9942	41.9587	42.0314	41.9999	41.8824	3.677-11
86	$2s2p^53d$	$^4F^o_{5/2}$			42.0775	42.0414	42.1135	42.0830	41.9626	3.450-11
87	$2s2p^53d$	$^4F^o_{3/2}$			42.1521	42.1161	42.1905	42.1589	42.0387	1.909-11
88	$2s2p^53d$	$^4D^o_{7/2}$			42.2121	42.1770	42.2404	42.2204	42.0850	2.897-11
89	$2s2p^5(^1P)3p$	$^2D_{3/2}$			42.2732	42.2418	42.2675	42.2594	42.1287	1.646-12
90	$2s2p^53d$	$^4D^o_{1/2}$			42.3243	42.2883	42.3572	42.3311	42.2035	4.572-12
91	$2s2p^5(^1P)3p$	$^2D_{5/2}$			42.3436	42.3095	42.3363	42.3263	42.1962	1.957-12
92	$2s2p^53d$	$^4D^o_{5/2}$			42.3491	42.3095	42.3746	42.3497	42.2201	2.657-11
93	$2s2p^53d$	$^4D^o_{3/2}$			42.3633	42.3246	42.3937	42.3709	42.2401	7.444-12
94	$2s2p^5(^3P)3d$	$^2F^o_{7/2}$			42.3700	42.3300	42.3888	42.3665	42.2308	2.915-11
95	$2s2p^5(^3P)3d$	$^2D^o_{5/2}$			42.4019	42.3651	42.4224	42.4079	42.2585	2.755-11
96	$2s2p^5(^1P)3p$	$^2P_{1/2}$			42.4522	42.4212	42.4358	42.4416	42.3088	2.255-12
97	$2s2p^5(^1P)3p$	$^2P_{3/2}$			42.4859	42.4532	42.4688	42.4724	42.3407	2.618-12
98	$2s2p^5(^3P)3d$	$^2D^o_{3/2}$			42.4946	42.4583	42.5160	42.5018	42.3507	2.525-12
99	$2s2p^5(^3P)3d$	$^2F^o_{5/2}$			42.5757	42.5349	42.5907	42.5751	42.4246	2.676-11
100	$2s2p^5(^1P)3p$	$^2S_{1/2}$			42.6749	42.6456	42.7496	42.7062	42.5135	7.520-12
101	$2s2p^5(^3P)3d$	$^2P^o_{1/2}$			42.7307	42.6969	42.7642	42.7443	42.5888	1.981-13
102	$2s2p^5(^3P)3d$	$^2P^o_{3/2}$			42.9165	42.8747	42.9294	42.9221	42.7626	1.912-13

NIST: http://www.nist.gov/pml/data/asd.cfm; HFR: Earlier results of Jupén et al. [2]; GRASP1: Present results with the GRASP code for 501 level calculations *without* Breit and QED effects; GRASP2: Present results with the GRASP code for 501 level calculations *with* Breit and QED effects; FAC1: Present results with the FAC code for 113 level calculations; FAC2: Present results with the FAC code for 501 level calculations; FAC3: Present results with the FAC code for 38,089 level calculations.

The contributions of the Breit and QED effects on the energy levels of Sc XIII are not very significant, and are below 0.04 Ryd. However, these contributions have slightly lowered the energies and, subsequently, discrepancies with those of NIST have increased because comparatively there is a better match between the NIST and our energies obtained *without* them. Nevertheless, discrepancies between our results with GRASP (including the contributions from Breit and QED) and those of NIST are within 0.1 Ryd, and hence are highly satisfactory. Furthermore, there are no discrepancies in the level orderings between theory and measurements, and neither are there any ambiguities in level designations for this ion.

For most of the levels, there are no significant differences between the FAC1 and FAC2 energies, although the latter calculations include CI larger by more than a factor of four. However, for a few levels (such as 83 and 100), the differences are up to 0.04 Ryd, and energies in FAC2 are (mostly) lower. The same are the differences between the GRASP and FAC2 energies that include the same CI, but the latter ones are higher. Such small differences in energies between calculations with different codes are not uncommon and mainly arise due to the differences in algorithms, methodologies and formulations. Our FAC3 calculations include much larger CI and, as a result, the energies obtained are lower, by up to ∼0.2 Ryd, in comparison to those from FAC2. This has resulted in a better agreement with the GRASP energies. Although the FAC3 energies should be comparatively more accurate, differences with our GRASP or NIST are up to 0.25 Ryd—see, for example, levels 45–49 and 56–58. Since the FAC3 energies are the lowest, we consider our results with GRASP to be comparatively more accurate, with agreement within 0.1 Ryd (0.3%) with those of NIST, except for level 3 ($2s2p^6\ ^2S_{1/2}$) for which the discrepancy is 2%, or 0.14 Ryd. For this level, the energy calculated by Jönsson et al. [10] is closer to that of NIST because not only have they included a significantly larger CI, but their methodology is also different. Similarly, combining CI with the many-body perturbation theory (MBPT) approach, Gu [20] calculated the energy 6.945 Ryd, which is *lower* than that of NIST by only 0.014 Ryd, a tenth of the difference we have.

2.2. Sc XII

As for Sc XIII, for Sc XII, we have also performed a series of calculations with both GRASP and FAC. Our final calculations with GRASP include 3948 levels from 64 configurations, namely $2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$, $2s2p^64\ell$, $2s^22p^55\ell$, $2s2p^65\ell$, $2s^22p^56s/p/d$, $2s^22p^57s/p/d$, ($2s^22p^4$) 3s3p, 3s3d, 3p3d, $3s^2$, $3p^2$, $3d^2$, $3s4\ell$, $3s5\ell$, $3p4\ell$, $3p5\ell$, $3d4\ell$, and $3d5\ell$. Similarly, with FAC, we have performed mainly three sets of calculations, which are: (i) FAC1, which includes 3948 levels of the same configurations as in GRASP, (ii) FAC2, which includes 17 729 levels arising from all possible combinations of 2*8, (2*7) 3*1, 4*1, 5*1, 6*1, 7*1, (2*6) 3*2, 3*1 4*1, 3*1 5*1, 3*1 6*1, and 3*1 7*1, and finally (iii) FAC3, which includes a total of 93,437 levels, the additional ones arising from (2*6) 4*1 5*1, 4*1 6*1, 4*1 7*1, 5*1 6*1, 5*1 7*1, 6*1 7*1, and 2*5 3*3. These calculations are on the same lines as considered for some other Ne-like ions [14,15].

In Table 2, we list our *final* energies from both GRASP and FAC for the lowest 125 levels because, beyond these from other configurations intermix, particularly from $2s^22p^56\ell$. However, energies for higher levels can be obtained from the author on request. In general, energies obtained in FAC1 (not listed here but discussed below) are lower than of GRASP by ∼0.1 Ryd, and both calculations include the same CI. This observation is similar to that noted earlier for Sc XIII. However, the FAC3 energies listed in Table 2 are lower than of GRASP by ∼0.2 Ryd, i.e., the effect of additional CI (by more than a factor of 20) is about 0.1 Ryd. In addition, for a few levels, such as 79–84, there are some (minor) differences in energy orderings, but overall there are no (major) discrepancies between calculations with two different codes. This result was expected and has been noted earlier for several ions, including some Ne-like [14,15], although some authors, such as [21], have shown differences of up to ∼2 Ryd, but their calculations are incorrect as discussed in [14,15] and further explained in [22,23]—see also [24] for many other examples of discrepancies. Although a good agreement between the two calculations in our work confirms the accuracy of the calculated energies, we discuss these further below.

Table 2. Energies (in Ryd) and lifetimes (τ, s) for the lowest 125 levels of Sc XII. $a \pm b \equiv a \times 10^{\pm b}$.

Index	Configuration	Level	GRASP	FAC	τ (GRASP)
1	$2s^22p^6$	$^1S_0$	0.0000	0.0000	....
2	$2s^22p^53s$	$^3P^o_2$	29.3855	29.2066	4.462-05
3	$2s^22p^53s$	$^3P^o_1$	29.4771	29.2951	4.228-12
4	$2s^22p^53s$	$^3P^o_0$	29.7278	29.5422	1.530-03
5	$2s^22p^53s$	$^1P^o_1$	29.8033	29.6144	2.977-12
6	$2s^22p^53p$	$^3S_1$	30.9051	30.7362	5.161-10
7	$2s^22p^53p$	$^3D_2$	31.1455	30.9717	3.044-10
8	$2s^22p^53p$	$^3D_3$	31.1574	30.9846	2.805-10
9	$2s^22p^53p$	$^3D_1$	31.2401	31.0644	2.816-10
10	$2s^22p^53p$	$^3P_2$	31.3076	31.1331	2.276-10
11	$2s^22p^53p$	$^1P_1$	31.4772	31.2961	3.104-10
12	$2s^22p^53p$	$^3P_0$	31.4838	31.3059	2.131-10
13	$2s^22p^53p$	$^3P_1$	31.5815	31.4010	2.383-10
14	$2s^22p^53p$	$^1D_2$	31.5802	31.3991	2.559-10
15	$2s^22p^53p$	$^1S_0$	32.5413	32.3164	5.725-11
16	$2s^22p^53d$	$^3P^o_0$	33.3120	33.1018	1.287-10
17	$2s^22p^53d$	$^3P^o_1$	33.3461	33.1362	3.549-11
18	$2s^22p^53d$	$^3P^o_2$	33.4151	33.2043	1.303-10
19	$2s^22p^53d$	$^3F^o_4$	33.4436	33.2375	1.278-10
20	$2s^22p^53d$	$^3F^o_3$	33.4876	33.2737	1.190-10
21	$2s^22p^53d$	$^3F^o_2$	33.5655	33.3496	1.142-10
22	$2s^22p^53d$	$^3D^o_3$	33.6145	33.3953	1.166-10
23	$2s^22p^53d$	$^3D^o_1$	33.7817	33.5589	1.357-12
24	$2s^22p^53d$	$^1D^o_2$	33.8489	33.6321	1.131-10
25	$2s^22p^53d$	$^3D^o_2$	33.8858	33.6592	1.151-10
26	$2s^22p^53d$	$^1F^o_3$	33.8933	33.6665	1.194-10
27	$2s^22p^53d$	$^1P^o_1$	34.2991	34.0503	1.331-13
28	$2s2p^63s$	$^3S_1$	36.5770	36.4646	1.004-11
29	$2s2p^63s$	$^1S_0$	36.9177	36.7847	1.554-11
30	$2s2p^63p$	$^3P^o_0$	38.2806	38.1830	1.064-11
31	$2s2p^63p$	$^3P^o_1$	38.2949	38.1970	6.973-12
32	$2s2p^63p$	$^3P^o_2$	38.3440	38.2460	1.033-11
33	$2s2p^63p$	$^1P^o_1$	38.4635	38.3613	8.246-13
34	$2s^22p^54s$	$^3P^o_2$	39.4229	39.2385	9.358-12
35	$2s^22p^54s$	$^1P^o_1$	39.4492	39.2665	4.976-12
36	$2s^22p^54s$	$^3P^o_0$	39.7631	39.5717	9.131-12
37	$2s^22p^54s$	$^3P^o_1$	39.7790	39.5889	5.632-12
38	$2s^22p^54p$	$^3S_1$	40.0442	39.8628	1.232-11
39	$2s^22p^54p$	$^3D_2$	40.0825	39.9043	1.056-11
40	$2s^22p^54p$	$^3D_3$	40.0825	39.9037	1.075-11
41	$2s^22p^54p$	$^1P_1$	40.1279	39.9477	1.098-11
42	$2s^22p^54p$	$^3P_2$	40.1497	39.9701	1.169-11
43	$2s^22p^54p$	$^3P_0$	40.3069	40.1259	1.233-11
44	$2s^22p^54p$	$^3D_1$	40.3850	40.2085	1.079-11
45	$2s^22p^54p$	$^1D_2$	40.4298	40.2543	1.128-11
46	$2s^22p^54p$	$^3P_1$	40.4623	40.2756	1.186-11
47	$2s2p^63d$	$^3D_3$	40.5465	40.4081	2.170-11
48	$2s2p^63d$	$^3D_1$	40.5616	40.4126	2.323-11
49	$2s2p^63d$	$^3D_2$	40.5614	40.4136	2.152-11
50	$2s^22p^54p$	$^1S_0$	40.7344	40.5575	1.427-11
51	$2s2p^63d$	$^1D_2$	40.7676	40.6156	1.983-11
52	$2s^22p^54d$	$^3P^o_0$	40.8897	40.7058	7.852-12
53	$2s^22p^54d$	$^3P^o_1$	40.9080	40.7234	6.962-12
54	$2s^22p^54d$	$^3F^o_4$	40.9328	40.7469	7.748-12
55	$2s^22p^54d$	$^3P^o_2$	40.9388	40.7529	7.898-12
56	$2s^22p^54d$	$^3F^o_3$	40.9524	40.7648	7.871-12
57	$2s^22p^54d$	$^1D^o_2$	40.9819	40.7928	8.035-12
58	$2s^22p^54d$	$^3D^o_3$	40.9966	40.8076	8.035-12

Table 2. *Cont.*

Index	Configuration	Level	GRASP	FAC	τ (GRASP)
59	$2s^22p^54d$	$^3D^o_1$	41.1063	40.9116	8.331-13
60	$2s^22p^54f$	$^3G_5$	41.2824	41.0918	3.184-12
61	$2s^22p^54f$	$^1G_4$	41.2829	41.0922	3.206-12
62	$2s^22p^54d$	$^3F^o_2$	41.2919	41.0986	7.908-12
63	$2s^22p^54f$	$^1F_3$	41.3078	41.1174	3.209-12
64	$2s^22p^54d$	$^3D^o_2$	41.3095	41.1062	3.215-12
65	$2s^22p^54f$	$^3F_4$	41.3006	41.1193	7.978-12
66	$2s^22p^54d$	$^1F^o_3$	41.3128	41.1177	7.893-12
67	$2s^22p^54f$	$^3F_2$	41.3262	41.1368	3.062-12
68	$2s^22p^54f$	$^3F_3$	41.3284	41.1388	2.968-12
69	$2s^22p^54f$	$^3D_1$	41.3386	41.1497	2.695-12
70	$2s^22p^54f$	$^3D_2$	41.3388	41.1502	2.801-12
71	$2s^22p^54d$	$^1P^o_1$	41.4470	41.2417	3.844-13
72	$2s^22p^54f$	$^3G_3$	41.6359	41.4388	3.193-12
73	$2s^22p^54f$	$^3G_4$	41.6383	41.4411	3.208-12
74	$2s^22p^54f$	$^1D_2$	41.6614	41.4647	3.059-12
75	$2s^22p^54f$	$^3D_3$	41.6638	41.4668	2.948-12
76	$2s^22p^55s$	$^3P^o_2$	43.6194	43.3963	1.163-11
77	$2s^22p^55s$	$^1P^o_1$	43.6353	43.4126	6.884-12
78	$2s^22p^55p$	$^3S_1$	43.9292	43.7080	1.432-11
79	$2s^22p^55p$	$^3D_2$	43.9556	43.7343	1.412-11
80	$2s^22p^55p$	$^3D_3$	43.9580	43.7362	1.455-11
81	$2s^22p^55p$	$^1P_1$	43.9727	43.7506	1.375-11
82	$2s^22p^55s$	$^3P^o_0$	43.9636	43.7332	1.161-11
83	$2s^22p^55p$	$^3P_2$	43.9820	43.7601	1.491-11
84	$2s^22p^55s$	$^3P^o_1$	43.9717	43.7416	7.711-12
85	$2s^22p^55p$	$^3P_0$	44.0864	43.8633	1.588-11
86	$2s^22p^55p$	$^3D_1$	44.2937	44.0642	1.381-11
87	$2s^22p^55p$	$^3P_1$	44.3076	44.0788	1.466-11
88	$2s^22p^55p$	$^1D_2$	44.3137	44.0849	1.454-11
89	$2s^22p^55d$	$^3P^o_0$	44.3373	44.1172	9.963-12
90	$2s^22p^55d$	$^3P^o_1$	44.3475	44.1267	9.039-12
91	$2s^22p^55d$	$^3F^o_4$	44.3578	44.1361	1.015-11
92	$2s^22p^55d$	$^3P^o_2$	44.3628	44.1408	1.013-11
93	$2s^22p^55d$	$^3F^o_3$	44.3676	44.1450	1.022-11
94	$2s^22p^55d$	$^1D^o_2$	44.3816	44.1577	1.038-11
95	$2s^22p^55d$	$^3D^o_3$	44.3883	44.1642	1.034-11
96	$2s^22p^55p$	$^1S_0$	44.4089	44.1797	1.608-11
97	$2s^22p^55d$	$^3D^o_1$	44.4555	44.2249	9.363-13
98	$2s^22p^55f$	$^3D_1$	44.5338	44.3169	5.510-12
99	$2s^22p^55f$	$^3G_5$	44.5342	44.3174	5.975-12
100	$2s^22p^55f$	$^1G_4$	44.5348	44.3180	6.015-12
101	$2s^22p^55f$	$^3D_2$	44.5363	44.3156	5.686-12
102	$2s^22p^55f$	$^3F_3$	44.5440	44.3161	5.722-12
103	$2s^22p^55f$	$^3F_2$	44.5458	44.3195	6.048-12
104	$2s^22p^55g$	$^3F^o_2$	44.5470	44.3291	1.129-11
105	$2s^22p^55f$	$^1F_3$	44.5470	44.3273	5.935-12
106	$2s^22p^55g$	$^3F^o_3$	44.5475	44.3231	1.131-11
107	$2s^22p^55f$	$^3F_4$	44.5479	44.3234	5.943-12
108	$2s^22p^55g$	$^1H^o_5$	44.5509	44.3193	1.129-11
109	$2s^22p^55g$	$^3H^o_6$	44.5513	44.3197	1.129-11
110	$2s^22p^55g$	$^3G^o_3$	44.5545	44.3301	1.133-11
111	$2s^22p^55g$	$^3G^o_4$	44.5548	44.3260	1.132-11
112	$2s^22p^55g$	$^1G^o_4$	44.5575	44.3313	1.132-11
113	$2s^22p^55g$	$^3G^o_5$	44.5579	44.3264	1.133-11
114	$2s^22p^55d$	$^3F^o_2$	44.7084	44.4787	1.026-11
115	$2s^22p^55d$	$^3D^o_2$	44.7113	44.4816	1.019-11

Table 2. *Cont.*

Index	Configuration	Level	GRASP	FAC	τ (GRASP)
116	$2s^22p^55d$	$^1F^o_3$	44.7189	44.4885	1.021-11
117	$2s^22p^55d$	$^1P^o_1$	44.7748	44.5376	8.700-13
118	$2s^22p^55f$	$^3G_3$	44.8831	44.6586	5.957-12
119	$2s^22p^55f$	$^3G_4$	44.8846	44.6589	5.986-12
120	$2s^22p^55f$	$^3D_3$	44.8870	44.6591	5.718-12
121	$2s^22p^55f$	$^1D_2$	44.8884	44.6644	5.946-12
122	$2s^22p^55g$	$^1F^o_3$	44.8973	44.6628	1.133-11
123	$2s^22p^55g$	$^3F^o_4$	44.8977	44.6593	1.132-11
124	$2s^22p^55g$	$^3H^o_4$	44.8982	44.6604	1.130-11
125	$2s^22p^55g$	$^3H^o_5$	44.8987	44.6597	1.130-11

GRASP: Present results with the GRASP code for 3948 level calculations; FAC: Present results with the FAC code for 93,437 level calculations.

As stated in Section 1, the only other energies available in the literature, but only for the lowest 27 levels, are by Cogordan and Lunell [5] and Jönsson et al. [10], who have also used (the different versions of) the GRASP code. Since experimental energies compiled by NIST are also available for a few levels of Sc XII, in Table 3, we compare different sets of energies for the lowest 37 levels, which belong to the $2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, and $2s^22p^54s$ configurations. The FAC1 and FAC2 energies differ at most by 0.2 Ryd (see levels 29–33), which indicates a small effect of additional CI included in the latter. However, further inclusion of CI in FAC3 is not of any (great) advantage because differences with FAC2 are below 0.02 Ryd, i.e., the results have converged. However, energy differences between the FAC3 and NIST are the largest, and are up to 0.3 Ryd for several levels, and those from the former are invariably lower. Therefore, as for Sc XIII, energies calculated with FAC for Sc XII too are comparatively less accurate. On the other hand, our calculations (and those of Cogordan and Lunell [5]) with GRASP compare well with those of NIST because the differences are within ∼0.1 Ryd (0.3%), with the measurements being (slightly) on the higher side. A notable exception is the level 15 ($2s^22p^53p$ $^1S_0$) for which the energy calculated by Cogordan and Lunell is (unusually) lower than our calculation by 0.14 Ryd. In all our calculations (with increasing CI) with the GRASP code, the energy obtained for this level is invariably higher, and the contributions of Breit and QED effects are only 0.02 Ryd. Therefore, the reason for this (comparatively) large difference is neither in the inclusion of (much) larger CI in our calculations nor in the modified version of the code adopted, but is due to the fact that they have treated this level separately in a different manner. Anyway, their calculated energy for this level is as much lower than NIST as ours is higher, and, therefore, the overall differences with measurements remain the same. Finally, the energies calculated by Jönsson et al. [10] are the most accurate because they have been able to produce results closer to those of NIST, for the same reasons as explained in Section 2.1 for Sc XIII.

Table 3. Comparison of energies (in Ryd) for the lowest 37 levels of Sc XII.

Index	Configuration	Level	FAC1	FAC2	FAC3	GRASP1	GRASP2	GRASP3	NIST
1	$2s^22p^6$	$^1S_0$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	$2s^22p^53s$	$^3P^o_2$	29.2619	29.2128	29.2066	29.4042	29.4787	29.3855	29.4811
3	$2s^22p^53s$	$^3P^o_1$	29.3592	29.3010	29.2951	29.5004	29.5695	29.4771	29.5720
4	$2s^22p^53s$	$^3P^o_0$	29.5982	29.5483	29.5422	29.7468	29.8215	29.7278	29.8233
5	$2s^22p^53s$	$^1P^o_1$	29.6831	29.6201	29.6144	29.8293	29.8956	29.8033	29.8970
6	$2s^22p^53p$	$^3S_1$	30.8156	30.7434	30.7362	30.9214	30.9967	30.9051	30.9960
7	$2s^22p^53p$	$^3D_2$	31.0546	30.9774	30.9717	31.1597	31.2317	31.1455	31.2312
8	$2s^22p^53p$	$^3D_3$	31.0678	30.9905	30.9846	31.1703	31.2434	31.1574	31.2431
9	$2s^22p^53p$	$^3D_1$	31.1490	31.0702	31.0644	31.2538	31.3235	31.2401	31.3234
10	$2s^22p^53p$	$^3P_2$	31.2157	31.1387	31.1331	31.3230	31.3942	31.3076	31.3940
11	$2s^22p^53p$	$^1P_1$	31.3817	31.3018	31.2961	31.4906	31.5606	31.4772	31.5598
12	$2s^22p^53p$	$^3P_0$	31.3885	31.3117	31.3059	31.4988	31.5678	31.4838	31.5681

Table 3. *Cont.*

Index	Configuration	Level	FAC1	FAC2	FAC3	GRASP1	GRASP2	GRASP3	NIST
13	$2s^22p^53p$	$^3P_1$	31.4852	31.4067	31.4010	31.5960	31.6668	31.5815	31.6662
14	$2s^22p^53p$	$^1D_2$	31.4831	31.4046	31.3991	31.5952	31.6669	31.5802	31.6662
15	$2s^22p^53p$	$^1S_0$	32.4021	32.3332	32.3164	32.4017	32.4890	32.5413	32.4845
16	$2s^22p^53d$	$^3P^o_0$	33.1852	33.1085	33.1018	33.3191	33.3960	33.3120	
17	$2s^22p^53d$	$^3P^o_1$	33.2200	33.1429	33.1362	33.3534	33.4287	33.3461	33.4302
18	$2s^22p^53d$	$^3P^o_2$	33.2889	33.2110	33.2043	33.4229	33.4966	33.4151	33.4980
19	$2s^22p^53d$	$^3F^o_4$	33.3187	33.2445	33.2375	33.4556	33.5222	33.4436	33.5237
20	$2s^22p^53d$	$^3F^o_3$	33.3577	33.2807	33.2737	33.5008	33.5636	33.4876	33.5650
21	$2s^22p^53d$	$^3F^o_2$	33.4356	33.3565	33.3496	33.5772	33.6396	33.5655	33.6413
22	$2s^22p^53d$	$^3D^o_3$	33.4844	33.4020	33.3953	33.6274	33.6874	33.6145	33.6887
23	$2s^22p^53d$	$^3D^o_1$	33.6480	33.5660	33.5589	33.7940	33.8517	33.7817	33.8510
24	$2s^22p^53d$	$^1D^o_2$	33.7188	33.6389	33.6321	33.8605	33.9227	33.8489	33.9238
25	$2s^22p^53d$	$^3D^o_2$	33.7487	33.6658	33.6592	33.8458	33.9598	33.8858	33.9608
26	$2s^22p^53d$	$^1F^o_3$	33.7549	33.6732	33.6665	33.9062	33.9674	33.8933	33.9682
27	$2s^22p^53d$	$^1P^o_1$	34.1446	34.0606	34.0503	34.3009	34.3355	34.2991	34.3300
28	$2s2p^63s$	$^3S_1$	36.6268	36.4760	36.4646			36.5770	
29	$2s2p^63s$	$^1S_0$	36.9957	36.7993	36.7847			36.9177	
30	$2s2p^63p$	$^3P^o_0$	38.3366	38.1944	38.1830			38.2806	
31	$2s2p^63p$	$^3P^o_1$	38.3507	38.2084	38.1970			38.2949	38.2550
32	$2s2p^63p$	$^3P^o_2$	38.3981	38.2575	38.2460			38.3440	
33	$2s2p^63p$	$^1P^o_1$	38.5280	38.3721	38.3613			38.4635	38.4100
34	$2s^22p^54s$	$^3P^o_2$	39.3200	39.2610	39.2385			39.4229	39.5248
35	$2s^22p^54s$	$^1P^o_1$	39.3463	39.2892	39.2665			39.4492	39.5430
36	$2s^22p^54s$	$^3P^o_0$	39.6538	39.5950	39.5717			39.7631	
37	$2s^22p^54s$	$^3P^o_1$	39.6702	39.6123	39.5889			39.7790	39.9030

FAC1: Present results with the FAC code for 3948 level calculations; FAC2: Present results with the FAC code for 17,729 level calculations; FAC3: Present results with the FAC code for 93,437 level calculations; GRASP1: Earlier results of Cogordan and Lunell [5] with the GRASP code; GRASP2: Earlier results of Jönsson et al. [10] with the GRASP code; GRASP3: Present results with the GRASP code for 3948 level calculations; NIST: http://www.nist.gov/pml/data/asd.cfm.

2.3. *Y XXX*

For Y XXX, we have performed similar calculations with GRASP and FAC as for Sc XII, described in Section 2.2. In Table 4, we list our *final* results with both these codes for the lowest 139 levels, as beyond these is an intermix from other configurations, such as $2s^22p^56\ell$. However, energies for higher levels can be obtained from the author on request. As stated in Section 1, similar results for some levels are available in the literature by Zhang and Sampson [7] and Hagelstein and Jung [6], who have used the Dirac–Fock–Slater (DFS) and YODA codes, respectively. The GRASP results are listed with inclusion (GRASP1) and exclusion (GRASP2) of Breit and QED effects because Y XXX is a comparatively heavy ion, and their net effect is to lower the energies by a maximum of 0.4 Ryd. Their effect is comparatively more noticeable on higher levels than the lower ones, and the maximum is on the ground level, i.e., 5.60 Ryd (3.25 + 2.35). The DFS energies, available for 89 levels, are closer to the GRASP2 results, which indicates the neglect of higher order relativistic effects from the calculations. The other results from YODA, although for only the lowest 37 levels, are closer to GRASP1 and agree within 0.1 Ryd, which is highly satisfactory. However, as for the other two ions, the corresponding results with FAC are the lowest among those listed in Table 4, although differing by a maximum of 0.2 Ryd with GRASP1. Before drawing our conclusion, we make a few other comparisons below.

In Table 5, we compare our GRASP results with those of Cogordan and Lunell [5] and Quinet et al. [8], who have used the same code but of different versions. Also included in the table are our results from three calculations with FAC, with increasing CI. All three sets of energies agree within 0.2 Ryd (see level 29) and hence the differences are insignificant, i.e., $<$0.1%. Similarly, all calculations with GRASP agree within 0.1 Ryd and hence provide confidence in our results listed in Table 4. Since the FAC energies are the lowest, irrespective of the level of CI, these results are assessed to be comparatively less accurate, and therefore our results obtained with the GRASP should be considered to be more accurate, and perhaps the best available to date for a larger number of levels. Further accuracy of our energy levels can be confirmed by the measurements, which, unfortunately, are not yet available for the levels of Y XXX.

Table 4. Energies (in Ryd) and lifetimes (τ, s) for the lowest 139 levels of Y XXX. $a \pm b \equiv a \times 10^{\pm b}$.

Index	Configuration	Level	GRASP1	GRASP2	FAC	DFS	YODA	τ (GRASP1)
1	$2s^22p^6$	$^1S_0$	0.0000	0.0000	0.0000	0.0000	0.0000	....
2	$2s^22p^53s$	$^3P^o_2$	146.6987	146.8657	146.5497	146.8576	146.8047	8.827-08
3	$2s^22p^53s$	$^1P^o_1$	146.9606	147.1241	146.8078	147.1295	147.0678	1.283-13
4	$2s^22p^53p$	$^3S_1$	150.9658	151.1208	150.8223	151.0984	151.0374	1.067-10
5	$2s^22p^53p$	$^3D_2$	151.1804	151.3472	151.0345	151.3336	151.2476	4.442-11
6	$2s^22p^53p$	$^3D_3$	152.4685	152.6663	152.3230	152.6493	152.5405	4.083-11
7	$2s^22p^53p$	$^1P_1$	152.4932	152.6816	152.3437	152.6640	152.5647	4.749-11
8	$2s^22p^53s$	$^3P^o_0$	152.4791	152.7338	152.3099	152.7375	152.6132	1.805-07
9	$2s^22p^53s$	$^3P^o_1$	152.6077	152.8713	152.4363	152.8771	152.7433	1.889-13
10	$2s^22p^53p$	$^3P_2$	152.8584	153.0399	152.7116	153.0314	152.9293	2.449-11
11	$2s^22p^53p$	$^3P_0$	154.2837	154.4569	154.1154	154.4647	154.3669	1.989-11
12	$2s^22p^53p$	$^3D_1$	156.8517	157.1167	156.6846	157.1106	156.9475	1.010-10
13	$2s^22p^53d$	$^3P^o_0$	157.6799	157.8546	157.5000	157.8309	157.7471	3.221-11
14	$2s^22p^53d$	$^3P^o_1$	157.8890	158.0863	157.7075	158.0661	157.9573	3.807-12
15	$2s^22p^53d$	$^3F^o_3$	158.1738	158.3932	157.9895	158.3822	158.2447	2.864-11
16	$2s^22p^53d$	$^3D^o_2$	158.2712	158.4762	158.0866	158.4557	158.3395	3.116-11
17	$2s^22p^53d$	$^3F^o_4$	158.2876	158.5230	158.1143	158.5071	158.3461	4.574-11
18	$2s^22p^53p$	$^3P_1$	158.3146	158.5880	158.1492	158.5806	158.4160	3.794-11
19	$2s^22p^53p$	$^1D_2$	158.4251	158.7151	158.2578	158.7129	158.5262	2.562-11
20	$2s^22p^53d$	$^1D^o_2$	158.5283	158.7396	158.3391	158.7202	158.6004	3.485-11
21	$2s^22p^53p$	$^1S_0$	158.6252	158.8512	158.4291	158.8893	158.7342	1.943-11
22	$2s^22p^53d$	$^3D^o_3$	158.8049	159.0240	158.6145	159.0142	158.8812	4.014-11
23	$2s^22p^53d$	$^3D^o_1$	159.7700	159.9925	159.5589	159.9991	159.8683	8.547-15
24	$2s^22p^53d$	$^3F^o_2$	163.9104	164.2167	163.7151	164.2106	164.0077	2.803-11
25	$2s^22p^53d$	$^3P^o_2$	164.2275	164.5414	164.0182	164.5340	164.3245	4.173-11
26	$2s^22p^53d$	$^1F^o_3$	164.3548	164.6758	164.1453	164.6736	164.4495	4.267-11
27	$2s^22p^53d$	$^1P^o_1$	164.8886	165.2049	164.6642	165.2175	164.9992	7.820-15
28	$2s2p^63s$	$^3S_1$	167.5933	167.8473	167.5051	167.8635	167.6790	2.216-12
29	$2s2p^63s$	$^1S_0$	168.4649	168.7070	168.3525	168.7381	168.5500	3.028-12
30	$2s2p^63p$	$^3P^o_0$	171.9546	172.1943	171.8826	172.2072	172.0073	2.413-12
31	$2s2p^63p$	$^3P^o_1$	172.0393	172.2913	171.9655	172.3028	172.0918	1.180-13
32	$2s2p^63p$	$^3P^o_2$	173.3963	173.6725	173.3240	173.6846	173.4560	2.304-12
33	$2s2p^63p$	$^1P^o_1$	173.6114	173.8890	173.5349	173.9051	173.6669	3.951-14
34	$2s2p^63d$	$^3D_1$	178.8170	179.0985	178.7101	179.1014	178.8809	2.685-12
35	$2s2p^63d$	$^3D_2$	178.8986	179.1968	178.7914	179.1970	178.9632	2.541-12
36	$2s2p^63d$	$^3D_3$	179.1053	179.4192	178.9983	179.4248	179.1624	2.585-12
37	$2s2p^63d$	$^1D_2$	179.7476	180.0497	179.6257	180.0789	179.8210	1.706-12
38	$2s^22p^54s$	$^3P^o_2$	199.3165	199.5290	199.1716	199.5414		3.442-13
39	$2s^22p^54s$	$^1P^o_1$	199.4034	199.6142	199.2606	199.6296		1.803-13
40	$2s^22p^54p$	$^3S_1$	201.0886	201.2950	200.9476	201.3053		3.072-13
41	$2s^22p^54p$	$^3D_2$	201.1477	201.3587	201.0071	201.3641		3.033-13
42	$2s^22p^54p$	$^3D_3$	201.6754	201.8994	201.5336	201.9080		3.378-13
43	$2s^22p^54p$	$^1P_1$	201.6926	201.9130	201.5496	201.9227		3.317-13
44	$2s^22p^54p$	$^3P_2$	201.8149	202.0323	201.6736	202.0403		3.445-13
45	$2s^22p^54p$	$^1S_0$	202.4018	202.6089	202.2643	202.6210		3.651-13
46	$2s^22p^54d$	$^3P^o_0$	203.6528	203.8698	203.5107	203.8851		1.740-13
47	$2s^22p^54d$	$^3P^o_1$	203.7330	203.9577	203.5899	203.9733		1.709-13
48	$2s^22p^54d$	$^3F^o_3$	203.8229	204.0551	203.6770	204.0615		1.763-13
49	$2s^22p^54d$	$^3D^o_2$	203.8692	204.0950	203.7236	204.1056		1.763-13
50	$2s^22p^54d$	$^3F^o_4$	203.8863	204.1251	203.7419	204.1350		1.740-13
51	$2s^22p^54d$	$^1D^o_2$	203.9686	204.1992	203.8208	204.2085		1.754-13
52	$2s^22p^54d$	$^3D^o_3$	204.0699	204.3017	203.9220	204.3114		1.762-13
53	$2s^22p^54d$	$^1P^o_1$	204.4392	204.6729	204.2800	204.6789		1.619-14
54	$2s^22p^54f$	$^3D_1$	205.0260	205.2616	204.8713	205.2816		8.126-14
55	$2s^22p^54f$	$^3G_4$	205.0516	205.2961	204.8970	205.3184		8.452-14
56	$2s^22p^54f$	$^3D_2$	205.0755	205.3135	204.9208	205.3331		8.218-14
57	$2s^22p^54f$	$^3G_5$	205.0973	205.3419	204.9425	205.3625		8.462-14
58	$2s^22p^54f$	$^3F_3$	205.1329	205.3729	204.9787	205.3919		8.392-14
59	$2s^22p^54f$	$^1D_2$	205.1513	205.3899	204.9965	205.4139		8.569-14

Table 4. *Cont.*

Index	Configuration	Level	GRASP1	GRASP2	FAC	DFS	YODA	τ (GRASP1)
60	$2s^22p^54f$	$^1F_3$	205.1659	205.4060	205.0108	205.4246		8.382-14
61	$2s^22p^54s$	$^3P^o_0$	205.1153	205.4217	204.9493	205.4433		3.427-13
62	$2s^22p^54f$	$^3F_4$	205.1953	205.4368	205.0410	205.4580		8.490-14
63	$2s^22p^54s$	$^3P^o_1$	205.1705	205.4783	205.0058	205.5021		3.381-13
64	$2s^22p^54p$	$^3D_1$	206.9038	207.2126	206.7408	207.2293		2.999-13
65	$2s^22p^54p$	$^3P_0$	207.3845	207.6802	207.2255	207.7071		3.224-13
66	$2s^22p^54p$	$^3P_1$	207.4992	207.8124	207.3363	207.8320		3.411-13
67	$2s^22p^54p$	$^1D_2$	207.5333	207.8527	207.3708	207.8688		3.384-13
68	$2s^22p^54d$	$^3F^o_2$	209.5980	209.9242	209.4319	209.9488		1.763-13
69	$2s^22p^54d$	$^3P^o_2$	209.7364	210.0653	209.5701	210.0884		1.744-13
70	$2s^22p^54d$	$^1F^o_3$	209.7832	210.1147	209.6157	210.1325		1.750-13
71	$2s^22p^54d$	$^3D^o_1$	209.9192	210.2458	209.7448	210.2648		2.381-14
72	$2s^22p^54f$	$^3G_3$	210.8816	211.2201	210.7060	211.2571		8.423-14
73	$2s^22p^54f$	$^3F_2$	210.9115	211.2487	210.7362	211.2791		8.427-14
74	$2s^22p^54f$	$^1G_4$	210.9436	211.2829	210.7674	211.3159		8.492-14
75	$2s^22p^54f$	$^3D_3$	210.9487	211.2869	210.7725	211.3159		8.335-14
76	$2s2p^64s$	$^3S_1$	219.9878	220.2881	219.9299	220.3194		2.957-13
77	$2s2p^64s$	$^1S_0$	220.3037	220.5991	220.2466	220.6134		3.127-13
78	$2s2p^64p$	$^3P^o_0$	221.8067	222.1002	221.7550	222.1201		2.714-13
79	$2s2p^64p$	$^3P^o_1$	221.8169	222.1140	221.7623	222.1495		1.018-13
80	$2s2p^64p$	$^3P^o_2$	222.2897	222.5686	222.1888	222.7228		3.191-13
81	$2s2p^64p$	$^1P^o_1$	222.4682	222.7721	222.4021	222.7963		5.936-14
82	$2s^22p^55s$	$^1P^o_1$	222.6048	222.8365	222.4369			2.513-13
83	$2s^22p^55s$	$^3P^o_2$	222.6489	222.9041	222.5133			4.010-13
84	$2s^22p^55p$	$^3S_1$	223.4433	223.6654	223.2605			3.891-13
85	$2s^22p^55p$	$^3D_2$	223.4497	223.6750	223.2688			3.711-13
86	$2s^22p^55p$	$^3D_3$	223.7106	223.9432	223.5300			4.028-13
87	$2s^22p^55p$	$^1P_1$	223.7394	223.9689	223.5557			4.095-13
88	$2s^22p^55p$	$^3P_2$	223.7892	224.0166	223.6064			4.206-13
89	$2s^22p^55p$	$^1S_0$	224.0789	224.2965	223.8943			4.332-13
90	$2s2p^64d$	$^3D_1$	224.4288	224.7380	224.3693	224.7881		1.733-13
91	$2s2p^64d$	$^3D_2$	224.4779	224.7928	224.4184	224.8249		1.720-13
92	$2s2p^64d$	$^3D_3$	224.5842	224.9046	224.5246	224.9278		1.703-13
93	$2s^22p^55d$	$^3P^o_0$	224.6993	224.9276	224.5216			2.400-13
94	$2s^22p^55d$	$^3P^o_1$	224.7374	224.9689	224.5588			2.383-13
95	$2s^22p^55d$	$^3F^o_3$	224.7747	225.0091	224.5944			2.405-13
96	$2s^22p^55d$	$^3D^o_2$	224.7997	225.0306	224.6191			2.418-13
97	$2s^22p^55d$	$^3F^o_4$	224.8111	225.0491	224.6317			2.401-13
98	$2s^22p^55d$	$^1D^o_2$	224.8502	225.0839	224.6686			2.407-13
99	$2s2p^64d$	$^1D_2$	224.7977	225.1145	224.7342	225.1336		1.696-13
100	$2s^22p^55d$	$^3D^o_3$	224.8972	225.1308	224.7150			2.409-13
101	$2s^22p^55d$	$^1P^o_1$	225.0872	225.3180	224.8959			3.097-14
102	$2s^22p^55g$	$^3F^o_2$	225.3178	225.5788	225.1566			2.050-13
103	$2s^22p^55g$	$^3F^o_3$	225.3502	225.6094	225.1846			2.157-13
104	$2s^22p^55f$	$^3G_4$	225.3857	225.6287	225.2042			1.608-13
105	$2s^22p^55f$	$^3D_1$	225.3960	225.6370	225.2177			1.486-13
106	$2s^22p^55f$	$^3G_5$	225.4076	225.6509	225.2261			1.611-13
107	$2s^22p^55f$	$^3D_2$	225.4161	225.6579	225.2372			1.515-13
108	$2s^22p^55f$	$^3F_3$	225.4264	225.6673	225.2451			1.586-13
109	$2s^22p^55g$	$^3G^o_3$	225.4225	225.6782	225.2485			2.272-13
110	$2s^22p^55f$	$^1D_2$	225.4457	225.6869	225.2651			1.602-13
111	$2s^22p^55g$	$^3G^o_4$	225.4377	225.6930	225.2631			2.281-13
112	$2s^22p^55f$	$^1F_3$	225.4515	225.6938	225.2713			1.551-13
113	$2s^22p^55f$	$^3F_4$	225.4566	225.6982	225.2750			1.603-13
114	$2s^22p^55g$	$^1H^o_5$	225.4899	225.7330	225.2931			2.882-13
115	$2s^22p^55g$	$^3H^o_6$	225.5069	225.7498	225.3100			2.889-13
116	$2s^22p^55g$	$^1G^o_4$	225.5151	225.7571	225.3186			2.882-13
117	$2s^22p^55g$	$^3G^o_5$	225.5310	225.7730	225.3345			2.892-13
118	$2s2p^64f$	$^3F^o_3$	225.7962	226.1104	225.7044	226.0597		8.881-14
119	$2s2p^64f$	$^3F^o_4$	225.8311	226.1473	225.7417	226.1111		8.798-14
120	$2s2p^64f$	$^3F^o_2$	225.8669	226.1719	225.7639	226.0523		9.089-14
121	$2s2p^64f$	$^1F^o_3$	225.9203	226.2297	225.8217	226.1332		8.967-14
122	$2s^22p^55s$	$^3P^o_0$	228.3506	228.6719	228.1423			4.345-13
123	$2s^22p^55s$	$^3P^o_1$	228.3696	228.6922	228.1616			3.699-13
124	$2s^22p^55p$	$^3D_1$	229.2465	229.5683	229.2483			3.776-13
125	$2s^22p^55p$	$^3P_0$	229.4556	229.7686	229.0393			3.932-13
126	$2s^22p^55p$	$^3P_1$	229.5449	229.8690	229.3380			4.238-13

Table 4. *Cont.*

Index	Configuration	Level	GRASP1	GRASP2	FAC	DFS	YODA	τ (GRASP1)
127	$2s^22p^55p$	$^1D_2$	229.5601	229.8870	229.3535			4.207-13
128	$2s^22p^55d$	$^3F^o_2$	230.5663	230.8966	230.3626			2.415-13
129	$2s^22p^55d$	$^3P^o_2$	230.6384	230.9698	230.4346			2.397-13
130	$2s^22p^55d$	$^1F^o_3$	230.6603	230.9929	230.4558			2.407-13
131	$2s^22p^55d$	$^3D^o_1$	230.7145	231.0425	230.5047			4.944-14
132	$2s^22p^55f$	$^3G_3$	231.2020	231.5406	230.9968			1.599-13
133	$2s^22p^55f$	$^3F_2$	231.2205	231.5584	231.0153			1.598-13
134	$2s^22p^55f$	$^1G_4$	231.2348	231.5740	231.0291			1.612-13
135	$2s^22p^55f$	$^3D_3$	231.2366	231.5751	231.0308			1.576-13
136	$2s^22p^55g$	$^3H^o_4$	231.3059	231.6452	231.0853			2.883-13
137	$2s^22p^55g$	$^1F^o_3$	231.3132	231.6521	231.0928			2.839-13
138	$2s^22p^55g$	$^3H^o_5$	231.3233	231.6626	231.1026			2.891-13
139	$2s^22p^55g$	$^3F^o_4$	231.3301	231.6691	231.1097			2.844-13

GRASP1: Present results with the GRASP code for 3948 level calculations *including* Breit and QED effects; GRASP2: Present results with the GRASP code for 3948 level calculations *excluding* Breit and QED effects; FAC: Present results with the FAC code for 93,437 level calculations; DFS: Earlier results of Zhang and Sampson [7]; YODA: Earlier results of Hagelstein and Jung [6].

Table 5. Comparison of energies (in Ryd) for the lowest 37 levels of Y XXX.

Index	Configuration	Level	FAC1	FAC2	FAC3	GRASP1	GRASP2	GRASP3
1	$2s^22p^6$	$^1S_0$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	$2s^22p^53s$	$^3P^o_2$	146.6164	146.5697	146.5497	146.7014		146.6987
3	$2s^22p^53s$	$^1P^o_1$	146.8884	146.8272	146.8078	146.9787		146.9606
4	$2s^22p^53p$	$^3S_1$	150.9125	150.8425	150.8223	150.9653	151.0112	150.9658
5	$2s^22p^53p$	$^3D_2$	151.1260	151.0538	151.0345	151.1747		151.1804
6	$2s^22p^53p$	$^3D_3$	152.4161	152.3427	152.3230	152.4651	152.5129	152.4685
7	$2s^22p^53p$	$^1P_1$	152.4397	152.3634	152.3437	152.4908	152.5414	152.4932
8	$2s^22p^53s$	$^3P^o_0$	152.3800	152.3298	152.3099	152.4813	152.5560	152.4791
9	$2s^22p^53s$	$^3P^o_1$	152.5137	152.4558	152.4363	152.6247		152.6077
10	$2s^22p^53p$	$^3P_2$	152.8034	152.7307	152.7116	152.8575		152.8584
11	$2s^22p^53p$	$^3P_0$	154.2124	154.1432	154.1154	154.2961	154.3980	154.2837
12	$2s^22p^53p$	$^3D_1$	156.7825	156.7041	156.6846	156.8470	156.9004	156.8517
13	$2s^22p^53d$	$^3P^o_0$	157.5915	157.5213	157.5000	157.6708	157.7660	157.6799
14	$2s^22p^53d$	$^3P^o_1$	157.8001	157.7287	157.7075	157.8813		157.8890
15	$2s^22p^53d$	$^3F^o_3$	158.0818	158.0112	157.9895	158.1763	158.2056	158.1738
16	$2s^22p^53d$	$^3D^o_2$	158.1807	158.1077	158.0866	158.2663	158.2950	158.2712
17	$2s^22p^53d$	$^3F^o_4$	158.2009	158.1363	158.1143	158.2879	158.3356	158.2876
18	$2s^22p^53p$	$^3P_1$	158.2446	158.1690	158.1492	158.3102	158.3604	158.3146
19	$2s^22p^53p$	$^1D_2$	158.3547	158.2770	158.2578	158.4209		158.4251
20	$2s^22p^53d$	$^1D^o_2$	158.4372	158.3602	158.3391	158.5266	158.5801	158.5283
21	$2s^22p^53p$	$^1S_0$	158.5336	158.4648	158.4291	158.5319	158.5608	158.6252
22	$2s^22p^53d$	$^3D^o_3$	158.7122	158.6354	158.6145	158.8041	158.8350	158.8049
23	$2s^22p^53d$	$^3D^o_1$	159.6610	159.5862	159.5589	159.7764		159.7700
24	$2s^22p^53d$	$^3F^o_2$	163.8100	163.7367	163.7151	163.9070	163.9513	163.9104
25	$2s^22p^53d$	$^3P^o_2$	164.1176	164.0390	164.0182	164.2192	164.2507	164.2275
26	$2s^22p^53d$	$^1F^o_3$	164.2434	164.1664	164.1453	164.3523	164.3840	164.3548
27	$2s^22p^53d$	$^1P^o_1$	164.7694	164.6913	164.6642	164.8795		164.8886
28	$2s2p^63s$	$^3S_1$	167.6548	167.5336	167.5051			167.5933
29	$2s2p^63s$	$^1S_0$	168.5527	168.3882	168.3525			168.4649
30	$2s2p^63p$	$^3P^o_0$	172.0201	171.9109	171.8826			171.9546
31	$2s2p^63p$	$^3P^o_1$	172.1062	171.9936	171.9655			172.0393
32	$2s2p^63p$	$^3P^o_2$	173.4597	173.3526	173.3240			173.3963
33	$2s2p^63p$	$^1P^o_1$	173.6801	173.5627	173.5349			173.6114
34	$2s2p^63d$	$^3D_1$	178.8518	178.7405	178.7101			178.8170
35	$2s2p^63d$	$^3D_2$	178.9334	178.8218	178.7914			178.8986
36	$2s2p^63d$	$^3D_3$	179.1391	179.0286	178.9983			179.1053
37	$2s2p^63d$	$^1D_2$	179.7807	179.6561	179.6257			179.7476

FAC1: Present results with the FAC code for 3948 level calculations; FAC2: Present results with the FAC code for 17 729 level calculations; FAC3: Present results with the FAC code for 93 437 level calculations; GRASP1: Earlier results of Cogordan and Lunell [5] with the GRASP code; GRASP2: Earlier results of Quinet et al. [8] with the GRASP code; GRASP3: Present results with the GRASP code for 3948 level calculations.

3. Radiative Rates

Our results for the A-values calculated with the GRASP code are listed in Tables 6–8 for the transitions in Sc XIII, Sc XII and Y XXX, respectively. For brevity, only resonance transitions, i.e., from the ground level, are listed here, but complete results for *all* transitions in ASCII format are available online as a supplementary material, and the indices for the lower (i) and upper (j) levels correspond to those listed in Tables 1, 2 and 4, for the respective ions. Furthermore, for the E1 transitions, we list absorption oscillator strength (f_{ij}) and line strength S (in atomic unit, 1 a.u. = 6.460 $\times$ 10^{-36} cm^2 esu^2) apart from the A-values, but only the latter parameter for other types of transitions, i.e., E2, M1 and M2. However, desired results for f- or S-values for these transitions can be easily obtained from the standard equations that have been listed in some of our earlier papers, but are also given below for a ready reference, i.e.,
for the electric dipole (E1) transitions

$$A_{ji} = \frac{2.0261 \times 10^{18}}{\omega_j \lambda_{ji}^3} S^{E1} \quad \text{and} \quad f_{ij} = \frac{303.75}{\lambda_{ji} \omega_i} S^{E1}, \tag{1}$$

for the magnetic dipole (M1) transitions

$$A_{ji} = \frac{2.6974 \times 10^{13}}{\omega_j \lambda_{ji}^3} S^{M1} \quad \text{and} \quad f_{ij} = \frac{4.044 \times 10^{-3}}{\lambda_{ji} \omega_i} S^{M1}, \tag{2}$$

for the electric quadrupole (E2) transitions

$$A_{ji} = \frac{1.1199 \times 10^{18}}{\omega_j \lambda_{ji}^5} S^{E2} \quad \text{and} \quad f_{ij} = \frac{167.89}{\lambda_{ji}^3 \omega_i} S^{E2}, \tag{3}$$

and for the magnetic quadrupole (M2) transitions

$$A_{ji} = \frac{1.4910 \times 10^{13}}{\omega_j \lambda_{ji}^5} S^{M2} \quad \text{and} \quad f_{ij} = \frac{2.236 \times 10^{-3}}{\lambda_{ji}^3 \omega_i} S^{M2}. \tag{4}$$

We also note here that f- and A-values are related as

$$f_{ij} = \frac{mc}{8\pi^2 e^2} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji}, \tag{5}$$

where m and e are the electron mass and charge, respectively, c is the velocity of light, λ_{ji} is the transition wavelength in Å, and ω_i and ω_j are the statistical weights of the lower i and upper j levels, respectively. This relationship is the same irrespective of the type of a transition, and λ_{ji} are also listed in Tables 6–8 for all possible transitions.

Assessing the accuracy of our calculated results for A-values (and other related parameters) is not straightforward. This is because no measurements are available for any transition of the ions concerned. However, limited theoretical results are available in the literature, which will perhaps be helpful for some accuracy assessments. For Sc XIII, Jönsson et al. [3] have listed A-values for the 1–3 E1 (4.635×10^{10} s^{-1}), 2–3 E1 (1.968×10^{10} s^{-1}), 1–2 M1 (9.773×10^2 s^{-1}), and 1–2 E2 (3.849×10^{-2} s^{-1}) transitions, which match very well (within 10%) with our corresponding results of 5.143×10^{10}, 2.193×10^{10}, 9.571×10^2, and 3.849×10^{-2} s^{-1}, respectively. However, this direct comparison of A-values is very limited. Some further assessments of accuracy can be made by comparing the length and velocity forms (i.e., the Babushkin and Coulomb gauges in the relativistic terms) of the A-values, and their ratio (R) for all E1 transitions are listed in Tables 6–8. Ideally, R should be closer to unity, but, in practice, it is not, particularly for the weak(er) transitions. For many strong transitions with $f \geq 0.1$, R is within 10% of unity as may be noted for the 1–49/52/55/56/59 transitions in Table 6. However, for 22 transitions (all with $f \leq 0.2$), R is up to 2 and examples include 9–26/78, 10–25/79 and 25–50/89. Similarly, for a few very weak transitions, R can be up to several orders of magnitude, and some examples are: 3–18 (f = 5.9 × 10^{-6}, R = 164), 3–21 (f = 3.8 × 10^{-4}, R = 83) and 3–23 (f = 4.0 × 10^{-5}, R = 357). For such weak transitions, the modelling of plasmas is not affected and similar large values of R are often noted for almost all ions in any large calculation.

Table 6. Transition wavelengths (λ_{ij} in Å), radiative rates (A_{ji} in s^{-1}), oscillator strengths (f_{ij}, dimensionless), and line strengths (S, in atomic units) for electric dipole (E1), and A_{ji} for E2, M1 and M2 transitions in Sc XIII. The last column gives the ratio R of the velocity and length forms of A(E1). $a \pm b \equiv a \times 10^{\pm b}$.

i	j	λ_{ij}	A_{ji}^{E1}	f_{ij}^{E1}	S^{E1}	A_{ji}^{E2}	A_{ij}^{M1}	A^{M2}	R
1	2	2.656 + 03	0.000 + 00	0.000 + 00	0.000 + 00	3.849 − 02	9.570 + 02	0.000 + 00	0.0 + 00
1	3	1.284 + 02	5.143 + 10	6.354 − 02	1.074 − 01	0.000 + 00	0.000 + 00	4.272 + 02	8.4 − 01
1	4	2.856 + 01	1.016 + 10	1.863 − 03	7.009 − 04	0.000 + 00	0.000 + 00	4.296 + 04	9.3 − 01
1	5	2.842 + 01	2.717 + 11	3.290 − 02	1.231 − 02	0.000 + 00	0.000 + 00	7.041 + 03	9.4 − 01
1	6	2.829 + 01	1.706 + 09	1.023 − 04	3.812 − 05	0.000 + 00	0.000 + 00	1.414 + 04	1.1 + 00
1	7	2.822 + 01	5.591 + 11	6.676 − 02	2.481 − 02	0.000 + 00	0.000 + 00	1.737 + 03	9.4 − 01
1	8	2.807 + 01	3.941 + 11	2.327 − 02	8.601 − 03	0.000 + 00	0.000 + 00	1.264 + 04	9.5 − 01
1	9	2.770 + 01	3.539 + 11	6.107 − 02	2.228 − 02	0.000 + 00	0.000 + 00	1.063 + 04	9.3 − 01
1	10	2.769 + 01	1.897 + 09	2.181 − 04	7.952 − 05	0.000 + 00	0.000 + 00	3.051 + 03	8.7 − 01
1	11	2.721 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.377 + 06	1.238 + 03	0.000 + 00	0.0 + 00
1	12	2.720 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.759 + 07	1.803 + 04	0.000 + 00	0.0 + 00
1	13	2.710 + 01	0.000 + 00	0.000 + 00	0.000 + 00	3.160 + 07	9.887 + 03	0.000 + 00	0.0 + 00
1	14	2.705 + 01	0.000 + 00	0.000 + 00	0.000 + 00	7.016 + 06	0.000 + 00	0.000 + 00	0.0 + 00
1	15	2.701 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.986 + 08	2.216 + 03	0.000 + 00	0.0 + 00
1	16	2.700 + 01	1.483 + 11	8.105 − 03	2.882 − 03	0.000 + 00	0.000 + 00	3.201 + 04	1.0 + 00
1	17	2.690 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.302 + 08	5.680 + 03	0.000 + 00	0.0 + 00
1	18	2.689 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.984 + 07	2.450 + 01	0.000 + 00	0.0 + 00
1	19	2.686 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.118 + 04	2.589 + 03	0.000 + 00	0.0 + 00
1	20	2.682 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.456 + 08	6.430 + 03	0.000 + 00	0.0 + 00
1	21	2.680 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.498 + 08	2.819 + 00	0.000 + 00	0.0 + 00
1	22	2.673 + 01	0.000 + 00	0.000 + 00	0.000 + 00	8.681 + 06	3.929 + 03	0.000 + 00	0.0 + 00
1	23	2.669 + 01	0.000 + 00	0.000 + 00	0.000 + 00	7.119 + 07	2.847 + 03	0.000 + 00	0.0 + 00
1	24	2.668 + 01	0.000 + 00	0.000 + 00	0.000 + 00	5.727 + 07	6.973 + 03	0.000 + 00	0.0 + 00
1	25	2.640 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.702 + 07	2.971 + 02	0.000 + 00	0.0 + 00
1	26	2.635 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.932 + 08	0.000 + 00	0.000 + 00	0.0 + 00
1	27	2.623 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.504 + 07	9.730 + 03	0.000 + 00	0.0 + 00
1	28	2.620 + 01	0.000 + 00	0.000 + 00	0.000 + 00	5.473 + 07	9.653 + 03	0.000 + 00	0.0 + 00
1	29	2.588 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.103 + 07	4.039 + 02	0.000 + 00	0.0 + 00
1	30	2.585 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.236 + 08	1.065 + 04	0.000 + 00	0.0 + 00
1	31	2.564 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.784 + 07	1.429 + 03	0.000 + 00	0.0 + 00
1	32	2.556 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.357 + 05	8.866 + 02	0.000 + 00	0.0 + 00
1	33	2.555 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	7.415 + 05	0.0 + 00
1	34	2.554 + 01	4.054 + 07	5.948 − 06	2.001 − 06	0.000 + 00	0.000 + 00	4.591 + 03	6.6 − 01
1	35	2.552 + 01	2.277 + 09	2.223 − 04	7.468 − 05	0.000 + 00	0.000 + 00	1.059 + 04	9.6 − 01
1	36	2.548 + 01	9.740 + 08	4.741 − 05	1.591 − 05	0.000 + 00	0.000 + 00	1.489 + 05	1.0 + 00
1	38	2.536 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.461 + 05	0.0 + 00
1	39	2.531 + 01	2.690 + 11	1.292 − 02	4.304 − 03	0.000 + 00	0.000 + 00	2.884 + 05	9.1 − 01
1	40	2.526 + 01	3.929 + 11	5.638 − 02	1.876 − 02	0.000 + 00	0.000 + 00	3.032 + 04	9.5 − 01
1	41	2.526 + 01	3.991 + 11	3.818 − 02	1.270 − 02	0.000 + 00	0.000 + 00	8.862 + 04	9.3 − 01
1	42	2.522 + 01	2.258 + 11	1.077 − 02	3.576 − 03	0.000 + 00	0.000 + 00	8.113 + 05	9.3 − 01
1	43	2.521 + 01	2.046 + 10	1.950 − 03	6.474 − 04	0.000 + 00	0.000 + 00	8.295 + 02	9.5 − 01
1	44	2.522 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.590 + 03	0.0 + 00
1	45	2.520 + 01	2.956 + 11	4.221 − 02	1.400 − 02	0.000 + 00	0.000 + 00	3.244 + 05	9.5 − 01
1	46	2.516 + 01	7.467 + 11	7.084 − 02	2.347 − 02	0.000 + 00	0.000 + 00	1.225 + 05	9.4 − 01
1	47	2.514 + 01	2.270 + 11	3.226 − 02	1.068 − 02	0.000 + 00	0.000 + 00	2.500 + 03	9.5 − 01
1	48	2.505 + 01	7.205 + 10	6.781 − 03	2.237 − 03	0.000 + 00	0.000 + 00	9.144 + 04	9.3 − 01
1	49	2.502 + 01	2.278 + 12	3.207 − 01	1.057 − 01	0.000 + 00	0.000 + 00	4.764 + 03	9.5 − 01
1	50	2.483 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	9.072 + 03	0.0 + 00
1	52	2.470 + 01	4.834 + 12	2.212 − 01	7.195 − 02	0.000 + 00	0.000 + 00	3.265 + 05	9.0 − 01
1	53	2.469 + 01	3.016 + 11	4.134 − 02	1.344 − 02	0.000 + 00	0.000 + 00	6.072 + 04	9.6 − 01

Table 6. *Cont.*

i	j	λ_{ij}	A_{ji}^{E1}	f_{ij}^{E1}	S^{E1}	A_{ji}^{E2}	A_{ij}^{M1}	A^{M2}	R
1	54	2.467 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.246 + 04	0.0 + 00
1	55	2.460 + 01	6.680 + 12	6.059 − 01	1.963 − 01	0.000 + 00	0.000 + 00	2.424 + 05	9.2 − 01
1	56	2.458 + 01	6.076 + 12	8.259 − 01	2.674 − 01	0.000 + 00	0.000 + 00	1.651 + 04	9.6 − 01
1	57	2.451 + 01	7.517 + 11	6.772 − 02	2.186 − 02	0.000 + 00	0.000 + 00	7.996 + 04	9.6 − 01
1	58	2.451 + 01	1.608 + 12	7.245 − 02	2.339 − 02	0.000 + 00	0.000 + 00	9.940 + 04	9.2 − 01
1	59	2.417 + 01	7.732 + 11	1.016 − 01	3.233 − 02	0.000 + 00	0.000 + 00	1.510 + 05	9.6 − 01
1	60	2.413 + 01	6.649 + 10	5.804 − 03	1.844 − 03	0.000 + 00	0.000 + 00	1.598 + 02	1.0 + 00
1	61	2.387 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.093 + 02	2.304 + 03	0.000 + 00	0.0 + 00
1	62	2.377 + 01	0.000 + 00	0.000 + 00	0.000 + 00	6.929 + 04	6.434 + 02	0.000 + 00	0.0 + 00
1	63	2.368 + 01	0.000 + 00	0.000 + 00	0.000 + 00	5.313 + 04	1.568 + 02	0.000 + 00	0.0 + 00
1	64	2.356 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.346 + 06	6.397 + 01	0.000 + 00	0.0 + 00
1	65	2.344 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.864 + 06	2.384 + 02	0.000 + 00	0.0 + 00
1	66	2.299 + 01	6.378 + 07	5.052 − 06	1.529 − 06	0.000 + 00	0.000 + 00	3.535 + 04	5.4 − 01
1	67	2.285 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.067 + 05	0.0 + 00
1	68	2.285 + 01	1.207 + 11	1.417 − 02	4.262 − 03	0.000 + 00	0.000 + 00	7.639 + 01	1.0 + 00
1	69	2.280 + 01	1.445 + 11	1.126 − 02	3.379 − 03	0.000 + 00	0.000 + 00	1.961 + 04	9.5 − 01
1	70	2.274 + 01	4.807 + 11	5.591 − 02	1.675 − 02	0.000 + 00	0.000 + 00	7.822 + 04	1.0 + 00
1	71	2.274 + 01	2.117 + 10	8.206 − 04	2.457 − 04	0.000 + 00	0.000 + 00	8.406 + 01	9.3 − 01
1	72	2.268 + 01	7.750 + 11	5.979 − 02	1.786 − 02	0.000 + 00	0.000 + 00	1.618 + 04	9.5 − 01
1	73	2.266 + 01	3.728 + 11	4.306 − 02	1.285 − 02	0.000 + 00	0.000 + 00	2.096 + 04	1.0 + 00
1	74	2.265 + 01	3.029 + 10	1.165 − 03	3.473 − 04	0.000 + 00	0.000 + 00	2.006 + 04	9.8 − 01
1	75	2.265 + 01	2.244 + 11	1.726 − 02	5.147 − 03	0.000 + 00	0.000 + 00	6.875 + 03	9.9 − 01
1	76	2.261 + 01	7.117 + 11	2.728 − 02	8.124 − 03	0.000 + 00	0.000 + 00	8.459 + 03	9.6 − 01
1	77	2.256 + 01	1.087 + 10	8.295 − 04	2.465 − 04	0.000 + 00	0.000 + 00	4.842 + 03	7.4 − 01
1	78	2.242 + 01	0.000 + 00	0.000 + 00	0.000 + 00	3.231 + 03	7.871 + 02	0.000 + 00	0.0 + 00
1	79	2.241 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.042 + 05	1.739 + 03	0.000 + 00	0.0 + 00
1	80	2.237 + 01	6.381 + 11	2.393 − 02	7.047 − 03	0.000 + 00	0.000 + 00	5.659 + 03	1.0 + 00
1	81	2.180 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.445 + 04	2.086 + 02	0.000 + 00	0.0 + 00
1	82	2.177 + 01	0.000 + 00	0.000 + 00	0.000 + 00	8.185 + 05	1.952 + 01	0.000 + 00	0.0 + 00
1	84	2.174 + 01	0.000 + 00	0.000 + 00	0.000 + 00	7.207 + 06	1.597 + 01	0.000 + 00	0.0 + 00
1	85	2.172 + 01	0.000 + 00	0.000 + 00	0.000 + 00	4.140 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	86	2.167 + 01	0.000 + 00	0.000 + 00	0.000 + 00	9.654 + 07	1.069 + 02	0.000 + 00	0.0 + 00
1	87	2.164 + 01	0.000 + 00	0.000 + 00	0.000 + 00	5.051 + 07	7.469 + 01	0.000 + 00	0.0 + 00
1	88	2.161 + 01	0.000 + 00	0.000 + 00	0.000 + 00	6.636 + 08	0.000 + 00	0.000 + 00	0.0 + 00
1	89	2.157 + 01	9.573 + 10	6.679 − 03	1.898 − 03	0.000 + 00	0.000 + 00	3.241 + 03	1.0 + 00
1	90	2.155 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.414 + 07	3.011 + 01	0.000 + 00	0.0 + 00
1	91	2.154 + 01	3.598 + 11	3.754 − 02	1.065 − 02	0.000 + 00	0.000 + 00	4.381 + 04	9.5 − 01
1	92	2.154 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.498 + 07	4.910 + 00	0.000 + 00	0.0 + 00
1	93	2.153 + 01	0.000 + 00	0.000 + 00	0.000 + 00	9.335 + 06	1.958 + 01	0.000 + 00	0.0 + 00
1	94	2.153 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.171 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	95	2.151 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.606 + 09	1.808 − 01	0.000 + 00	0.0 + 00
1	96	2.148 + 01	6.229 + 10	2.155 − 03	6.095 − 04	0.000 + 00	0.000 + 00	1.887 + 04	1.3 + 00
1	97	2.147 + 01	1.437 + 11	9.927 − 03	2.806 − 03	0.000 + 00	0.000 + 00	4.044 + 04	1.3 + 00
1	98	2.146 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.386 + 09	6.283 + 00	0.000 + 00	0.0 + 00
1	99	2.142 + 01	0.000 + 00	0.000 + 00	0.000 + 00	8.041 + 07	2.817 + 01	0.000 + 00	0.0 + 00
1	100	2.137 + 01	9.936 + 09	3.401 − 04	9.570 − 05	0.000 + 00	0.000 + 00	6.580 + 04	3.2 − 01
1	101	2.134 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.070 + 09	2.749 + 01	0.000 + 00	0.0 + 00
1	102	2.125 + 01	0.000 + 00	0.000 + 00	0.000 + 00	4.964 + 08	4.492 + 00	0.000 + 00	0.0 + 00

For Sc XII, A-values for all types of transitions, but only among the lowest 27 levels, have been reported by Jönsson et al. [10] and, therefore, in Table 9, we make comparisons for the E1 and E2 transitions from the lowest five to higher excited levels. Generally, for all E1 transitions, the agreement between the two calculations is within ∼20%, which is highly satisfactory. However, for three weak transitions, namely 2–11 (f = 1.2 × 10^{-4}), 3–13 (f = 1.2 × 10^{-4}) and 5–9 (f = 4.4 × 10^{-5}), discrepancies are up to a factor of two. As already stated above, accuracies for such weak transitions are often not reliable and hence any of the two calculations can be (in)correct. Similarly, for the comparatively weak E2 transitions, the two calculations agree within 20% for most, but discrepancies are up to a factor of two for four (2–24, 3–24, 3–25, and 5–20), whereas it is factor of four for one, i.e., 5–21 (f = 3.2 × 10^{-10}).

Similar comparisons for the M1 and M2 transitions are made in Table 10. There are no appreciable discrepancies for the M2 transitions (except for 1–25), but, for a few M1, the differences are up to two orders of magnitude, see in particular 2–18 for which our $f = 9.7 \times 10^{-13}$. Such weak transitions (and discrepancies between different calculations) do not affect the modelling, or the subsequent calculations of lifetimes, $\tau = 1.0/\Sigma_i A_{ji}$, which includes contributions from all types of transitions, i.e., E1, E2, M1, and M2. This is further confirmed by comparing our results for τ, included in Tables 6–8, for the lowest 27 levels of Sc XII in Table 11, with those of Hibbert et al. [9] and Jönsson et al. [10], for which the agreements are within 10% for most levels.

Table 7. Transition wavelengths (λ_{ij} in Å), radiative rates (A_{ji} in s^{-1}), oscillator strengths (f_{ij}, dimensionless), and line strengths (S, in atomic units) for electric dipole (E1), and A_{ji} for E2, M1 and M2 transitions in Sc XII. The last column gives the ratio R of the velocity and length forms of A(E1). $a \pm b \equiv a \times 10^{\pm b}$.

i	j	λ_{ij}	A^{E1}_{ji}	f^{E1}_{ij}	S^{E1}	A^{E2}_{ji}	A^{M1}_{ij}	A^{M2}	R
1	2	3.101 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.241 + 04	0.0 + 00
1	3	3.091 + 01	2.365 + 11	1.017 − 01	1.035 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.4 − 01
1	5	3.058 + 01	3.359 + 11	1.412 − 01	1.422 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.4 − 01
1	6	2.949 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	8.085 + 03	0.000 + 00	0.0 + 00
1	7	2.926 + 01	0.000 + 00	0.000 + 00	0.000 + 00	7.312 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	9	2.917 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.521 + 03	0.000 + 00	0.0 + 00
1	10	2.911 + 01	0.000 + 00	0.000 + 00	0.000 + 00	9.485 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	11	2.895 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.143 + 00	0.000 + 00	0.0 + 00
1	13	2.885 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.699 + 04	0.000 + 00	0.0 + 00
1	14	2.886 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.167 + 08	0.000 + 00	0.000 + 00	0.0 + 00
1	17	2.733 + 01	2.044 + 10	6.865 − 03	6.176 − 04	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	18	2.727 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.992 + 05	0.0 + 00
1	21	2.715 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.530 + 04	0.0 + 00
1	23	2.698 + 01	7.276 + 11	2.381 − 01	2.115 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	24	2.692 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.344 + 04	0.0 + 00
1	25	2.689 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.704 + 03	0.0 + 00
1	27	2.657 + 01	7.503 + 12	2.382 + 00	2.084 − 01	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	28	2.491 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.295 + 03	0.000 + 00	0.0 + 00
1	31	2.380 + 01	4.824 + 10	1.229 − 02	9.625 − 04	0.000 + 00	0.000 + 00	0.000 + 00	9.9 − 01
1	32	2.377 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	8.775 + 04	0.0 + 00
1	33	2.369 + 01	1.114 + 12	2.813 − 01	2.194 − 02	0.000 + 00	0.000 + 00	0.000 + 00	1.0 + 00
1	34	2.311 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.187 + 03	0.0 + 00
1	35	2.310 + 01	8.909 + 10	2.138 − 02	1.626 − 03	0.000 + 00	0.000 + 00	0.000 + 00	8.2 − 01
1	37	2.291 + 01	6.570 + 10	1.551 − 02	1.170 − 03	0.000 + 00	0.000 + 00	0.000 + 00	8.3 − 01
1	38	2.276 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.454 + 03	0.000 + 00	0.0 + 00
1	39	2.274 + 01	0.000 + 00	0.000 + 00	0.000 + 00	8.428 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	41	2.271 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.889 + 02	0.000 + 00	0.0 + 00
1	42	2.270 + 01	0.000 + 00	0.000 + 00	0.000 + 00	8.206 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	44	2.257 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.896 + 01	0.000 + 00	0.0 + 00
1	45	2.254 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.516 + 08	0.000 + 00	0.000 + 00	0.0 + 00
1	46	2.252 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.392 + 03	0.000 + 00	0.0 + 00
1	48	2.247 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.968 + 01	0.000 + 00	0.0 + 00
1	49	2.247 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.945 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	51	2.235 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.082 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	53	2.228 + 01	1.660 + 10	3.704 − 03	2.717 − 04	0.000 + 00	0.000 + 00	0.000 + 00	9.5 − 01
1	55	2.226 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.037 + 05	0.0 + 00
1	57	2.224 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.724 + 04	0.0 + 00
1	59	2.217 + 01	1.081 + 12	2.389 − 01	1.744 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.5 − 01
1	62	2.207 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.861 + 04	0.0 + 00
1	65	2.206 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.348 + 04	0.0 + 00
1	67	2.205 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.607 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	69	2.204 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.594 − 02	0.000 + 00	0.0 + 00
1	70	2.204 + 01	0.000 + 00	0.000 + 00	0.000 + 00	3.388 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	71	2.199 + 01	2.487 + 12	5.406 − 01	3.913 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.5 − 01
1	74	2.187 + 01	0.000 + 00	0.000 + 00	0.000 + 00	7.572 + 07	0.000 + 00	0.000 + 00	0.0 + 00

Table 7. *Cont.*

i	j	λ_{ij}	A^{E1}_{ji}	f^{E1}_{ij}	S^{E1}	A^{E2}_{ji}	A^{M1}_{ij}	A^{M2}	R
1	76	2.089 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	7.937 + 03	0.0 + 00
1	77	2.088 + 01	5.646 + 10	1.108 − 02	7.614 − 04	0.000 + 00	0.000 + 00	0.000 + 00	7.1 − 01
1	78	2.074 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.896 + 03	0.000 + 00	0.0 + 00
1	79	2.073 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.839 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	81	2.072 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.077 + 02	0.000 + 00	0.0 + 00
1	83	2.072 + 01	0.000 + 00	0.000 + 00	0.000 + 00	2.467 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	84	2.072 + 01	4.167 + 10	8.049 − 03	5.491 − 04	0.000 + 00	0.000 + 00	0.000 + 00	7.3 − 01
1	86	2.057 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.494 + 02	0.000 + 00	0.0 + 00
1	87	2.057 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.694 + 03	0.000 + 00	0.0 + 00
1	88	2.056 + 01	0.000 + 00	0.000 + 00	0.000 + 00	3.006 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	90	2.055 + 01	1.092 + 10	2.073 − 03	1.402 − 04	0.000 + 00	0.000 + 00	0.000 + 00	9.2 − 01
1	92	2.054 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.693 + 05	0.0 + 00
1	94	2.053 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.708 + 04	0.0 + 00
1	97	2.050 + 01	9.711 + 11	1.835 − 01	1.238 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.2 − 01
1	98	2.046 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.006 + 01	0.000 + 00	0.0 + 00
1	101	2.046 + 01	0.000 + 00	0.000 + 00	0.000 + 00	7.876 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	103	2.046 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.535 + 08	0.000 + 00	0.000 + 00	0.0 + 00
1	104	2.046 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.763 − 01	0.0 + 00
1	114	2.038 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	7.163 + 03	0.0 + 00
1	115	2.038 + 01	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.434 + 04	0.0 + 00
1	117	2.035 + 01	1.052 + 12	1.960 − 01	1.313 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.2 − 01
1	121	2.030 + 01	0.000 + 00	0.000 + 00	0.000 + 00	1.136 + 08	0.000 + 00	0.000 + 00	0.0 + 00

Table 8. Transition wavelengths (λ_{ij} in Å), radiative rates (A_{ji} in s^{-1}), oscillator strengths (f_{ij}, dimensionless), and line strengths (S, in atomic units) for electric dipole (E1), and A_{ji} for E2, M1 and M2 transitions in Y XXX. The last column gives the ratio R of the velocity and length forms of A(E1). $a \pm b \equiv a \times 10^{\pm b}$.

i	j	λ_{ij}	A^{E1}_{ji}	f^{E1}_{ij}	S^{E1}	A^{E2}_{ji}	A^{M1}_{ij}	A^{M2}	R
1	2	6.212 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.133 + 07	0.0 + 00
1	3	6.201 + 00	7.791 + 12	1.347 − 01	2.750 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	4	6.036 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.716 + 07	0.000 + 00	0.0 + 00
1	5	6.028 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.212 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	7	5.976 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.612 + 06	0.000 + 00	0.0 + 00
1	9	5.971 + 00	5.295 + 12	8.492 − 02	1.669 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	10	5.962 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.207 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	12	5.810 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	9.393 + 05	0.000 + 00	0.0 + 00
1	14	5.772 + 00	2.314 + 11	3.467 − 03	6.588 − 05	0.000 + 00	0.000 + 00	0.000 + 00	9.9 − 01
1	16	5.758 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.542 + 08	0.0 + 00
1	18	5.756 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.680 + 07	0.000 + 00	0.0 + 00
1	19	5.752 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.360 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	20	5.748 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.417 + 08	0.0 + 00
1	23	5.704 + 00	1.170 + 14	1.711 + 00	3.213 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.9 − 01
1	24	5.560 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.046 + 07	0.0 + 00
1	25	5.549 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.876 + 07	0.0 + 00
1	27	5.527 + 00	1.278 + 14	1.756 + 00	3.195 − 02	0.000 + 00	0.000 + 00	0.000 + 00	9.9 − 01
1	28	5.437 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.951 + 06	0.000 + 00	0.0 + 00
1	31	5.297 + 00	8.047 + 12	1.015 − 01	1.771 − 03	0.000 + 00	0.000 + 00	0.000 + 00	1.0 + 00
1	32	5.255 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.146 + 07	0.0 + 00
1	33	5.249 + 00	2.487 + 13	3.082 − 01	5.326 − 03	0.000 + 00	0.000 + 00	0.000 + 00	1.0 + 00
1	34	5.096 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.141 + 05	0.000 + 00	0.0 + 00
1	35	5.094 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.792 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	37	5.070 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.910 + 11	0.000 + 00	0.000 + 00	0.0 + 00
1	38	4.572 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.736 + 06	0.0 + 00
1	39	4.570 + 00	2.603 + 12	2.445 − 02	3.679 − 04	0.000 + 00	0.000 + 00	0.000 + 00	9.4 − 01
1	40	4.532 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.509 + 07	0.000 + 00	0.0 + 00
1	41	4.530 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.685 + 09	0.000 + 00	0.000 + 00	0.0 + 00

Table 8. *Cont.*

i	j	λ_{ij}	A^{E1}_{ji}	f^{E1}_{ij}	S^{E1}	A^{E2}_{ji}	A^{M1}_{ij}	A^{M2}	R
1	43	4.518 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.076 + 06	0.000 + 00	0.0 + 00
1	44	4.515 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.666 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	47	4.473 + 00	1.232 + 11	1.108 − 03	1.632 − 05	0.000 + 00	0.000 + 00	0.000 + 00	9.7 − 01
1	49	4.470 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.720 + 07	0.0 + 00
1	51	4.468 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.694 + 08	0.0 + 00
1	53	4.457 + 00	5.627 + 13	5.028 − 01	7.379 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	54	4.445 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.868 + 04	0.000 + 00	0.0 + 00
1	56	4.444 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.124 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	59	4.442 + 00	0.000 + 00	0.000 + 00	0.000 + 00	8.106 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	63	4.442 + 00	4.538 + 08	4.026 − 06	5.887 − 08	0.000 + 00	0.000 + 00	0.000 + 00	7.4 − 02
1	64	4.404 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	6.172 + 05	0.000 + 00	0.0 + 00
1	66	4.392 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	7.599 + 06	0.000 + 00	0.0 + 00
1	67	4.391 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.185 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	68	4.348 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.712 + 06	0.0 + 00
1	69	4.345 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.947 + 07	0.0 + 00
1	71	4.341 + 00	3.645 + 13	3.089 − 01	4.415 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.8 − 01
1	73	4.321 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.337 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	76	4.142 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.683 + 06	0.000 + 00	0.0 + 00
1	79	4.108 + 00	6.095 + 12	4.626 − 02	6.257 − 04	0.000 + 00	0.000 + 00	0.000 + 00	9.7 − 01
1	80	4.100 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.307 + 07	0.0 + 00
1	81	4.096 + 00	1.361 + 13	1.027 − 01	1.385 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.6 − 01
1	82	4.094 + 00	1.530 + 12	1.153 − 02	1.554 − 04	0.000 + 00	0.000 + 00	0.000 + 00	1.1 + 00
1	83	4.093 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.039 + 07	0.0 + 00
1	84	4.078 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	7.559 + 06	0.000 + 00	0.0 + 00
1	85	4.078 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.121 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	87	4.073 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.142 + 06	0.000 + 00	0.0 + 00
1	88	4.072 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.314 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	90	4.060 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.209 + 05	0.000 + 00	0.0 + 00
1	91	4.060 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.615 + 08	0.000 + 00	0.000 + 00	0.0 + 00
1	94	4.055 + 00	3.708 + 10	2.742 − 04	3.660 − 06	0.000 + 00	0.000 + 00	0.000 + 00	9.6 − 01
1	96	4.054 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.795 + 07	0.0 + 00
1	98	4.053 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.017 + 08	0.0 + 00
1	99	4.054 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.670 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	101	4.049 + 00	2.818 + 13	2.077 − 01	2.769 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.7 − 01
1	102	4.044 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	1.852 + 03	0.0 + 00
1	105	4.043 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.972 + 04	0.000 + 00	0.0 + 00
1	107	4.043 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.482 + 07	0.000 + 00	0.000 + 00	0.0 + 00
1	110	4.042 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.045 + 10	0.000 + 00	0.000 + 00	0.0 + 00
1	120	4.035 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	5.833 + 02	0.0 + 00
1	123	3.990 + 00	3.816 + 11	2.733 − 03	3.590 − 05	0.000 + 00	0.000 + 00	0.000 + 00	8.3 − 01
1	124	3.975 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.987 + 05	0.000 + 00	0.0 + 00
1	126	3.970 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	4.065 + 06	0.000 + 00	0.0 + 00
1	127	3.970 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.774 + 09	0.000 + 00	0.000 + 00	0.0 + 00
1	128	3.952 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.570 + 06	0.0 + 00
1	129	3.951 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	0.000 + 00	2.334 + 07	0.0 + 00
1	131	3.950 + 00	1.609 + 13	1.129 − 01	1.468 − 03	0.000 + 00	0.000 + 00	0.000 + 00	9.7 − 01
1	133	3.941 + 00	0.000 + 00	0.000 + 00	0.000 + 00	3.073 + 10	0.000 + 00	0.000 + 00	0.0 + 00

For Y XXX, the only results available in the literature for comparison purposes are the f-values of Zhang and Sampson [7] for E1 transitions from the ground level and these are compared in Table 12. For a few weak transitions, the differences are large, in particular for 1–63 ($2s^22p^6\ ^1S_0$ – $2s^22p^54s\ ^3P^o_1$), a spin changing inter-combination transition, for which our f-value is very small ($\sim10^{-6}$), and subsequently the discrepancy is of three orders of magnitude. However, such comparisons are very limited and hence cannot be confidently relied upon. In conclusion, on the basis of the (whatever possible) comparisons have been made for all three ions, our experience on a wide range of other ions, including F-like [4,13] and Ne-like [14,15], and considering that we have included a large CI as well as relativistic effects in generating wavefunctions, we assess the accuracy of our radiative rates to be about 20%, for a majority of strong transitions with $f \geq 0.1$.

Table 9. Comparison of *A*-values (s^{-1}) for some E1 and E2 transitions of Sc XII. $a \pm b \equiv a \times 10^{\pm b}$.

E1				E2			
I	**J**	**GRASP**	**GRASP2K**	**I**	**J**	**GRASP**	**GRASP2K**
1	3	2.365 + 11	2.287 + 11	1	7	7.312 + 07	7.120 + 07
1	5	3.359 + 11	3.194 + 11	1	10	9.485 + 07	9.295 + 07
1	17	2.044 + 10	2.134 + 10	1	14	1.167 + 08	1.148 + 08
1	23	7.276 + 11	8.057 + 11	2	16	2.080 + 05	2.031 + 05
1	27	7.503 + 12	6.955 + 12	2	17	1.941 + 05	1.896 + 05
2	6	1.663 + 09	1.656 + 09	2	18	1.449 + 05	1.412 + 05
2	7	1.523 + 09	1.488 + 09	2	19	2.415 + 05	2.345 + 05
2	8	3.566 + 09	3.474 + 09	2	20	1.114 + 05	1.050 + 05
2	9	4.716 + 08	4.470 + 08	2	21	7.334 + 04	7.196 + 04
2	10	2.548 + 09	2.466 + 09	2	22	1.517 + 05	1.500 + 05
2	11	6.904 + 06	3.371 + 06	2	23	3.611 + 04	3.392 + 04
2	13	7.042 + 08	6.743 + 08	2	24	8.309 + 03	5.663 + 03
2	14	1.582 + 08	1.505 + 08	2	25	3.946 + 04	3.876 + 04
3	6	2.152 + 08	2.138 + 08	2	26	1.954 + 04	1.841 + 04
3	7	1.687 + 09	1.641 + 09	2	27	1.531 + 03	1.714 + 03
3	9	3.017 + 09	2.936 + 09	3	17	1.527 + 04	1.473 + 04
3	10	1.644 + 09	1.612 + 09	3	18	6.446 + 04	6.357 + 04
3	11	5.256 + 07	4.151 + 07	3	20	1.297 + 05	1.279 + 05
3	12	3.794 + 09	3.754 + 09	3	21	1.707 + 05	1.644 + 05
3	13	4.289 + 06	6.717 + 06	3	22	1.086 + 05	1.011 + 05
3	14	1.604 + 08	1.471 + 08	3	23	2.610 + 05	2.567 + 05
3	15	6.657 + 09	5.401 + 09	3	24	2.902 + 03	2.114 + 03
4	6	3.258 + 07	3.229 + 07	3	25	3.672 + 01	1.934 + 00
4	9	6.182 + 07	5.744 + 07	3	26	1.303 + 04	1.334 + 04
4	11	1.884 + 09	1.526 + 09	3	27	1.127 + 05	9.381 + 04
4	13	1.884 + 09	1.901 + 09	4	18	8.533 + 03	7.901 + 03
5	6	2.666 + 07	2.651 + 07	4	21	9.462 + 03	8.622 + 03
5	7	1.877 + 06	1.417 + 06	4	24	1.308 + 05	1.147 + 05
5	9	7.315 + 05	1.588 + 06	4	25	1.063 + 05	1.161 + 05
5	10	1.068 + 08	1.011 + 08	5	17	3.377 + 03	3.162 + 03
5	11	1.529 + 09	1.538 + 09	5	18	3.234 + 03	2.876 + 03
5	12	8.997 + 08	8.253 + 08	5	20	8.139 + 00	3.477 + 01
5	13	1.605 + 09	1.499 + 09	5	21	2.163 + 01	8.742 + 01
5	14	3.472 + 09	3.394 + 09	5	22	1.625 + 04	1.561 + 04
5	15	1.081 + 10	9.160 + 09	5	23	2.365 + 04	1.994 + 05
				5	24	1.100 + 05	1.186 + 05
				5	25	1.267 + 05	1.097 + 05
				5	26	2.328 + 05	2.243 + 05
				5	27	3.928 + 05	3.671 + 05

GRASP: Present results with the GRASP code for 3948 level calculations; GRASP2K: Earlier results of Jönsson et al. [10] with the GRASP2K code.

Table 10. Comparison of *A*-values (s^{-1}) for some M1 and M2 transitions of Sc XII. $a \pm b \equiv a \times 10^{\pm b}$.

E1				E2			
I	**J**	**GRASP**	**GRASP2K**	**I**	**J**	**GRASP**	**GRASP2K**
1	6	8.085 + 03	8.399 + 03	1	2	2.241 + 04	2.101 + 04
1	9	1.521 + 03	1.489 + 03	1	18	5.992 + 05	6.093 + 05
1	11	4.143 + 00	5.307 − 01	1	21	6.530 + 04	6.544 + 04
1	13	1.699 + 04	1.720 + 04	1	24	6.344 + 04	5.909 + 04
2	3	1.336 + 01	1.293 + 01	1	25	1.705 + 03	4.340 + 03
2	5	9.001 + 02	0.129 + 02	2	6	3.133 − 01	3.078 − 01
2	17	6.678 + 00	1.452 + 01	2	8	6.485 − 01	6.301 − 01
2	18	1.267 − 01	2.492 + 01	2	9	8.744 − 01	8.605 − 01
2	21	9.622 − 02	1.307 − 01	2	10	1.556 + 00	1.525 + 00

Table 10. *Cont.*

E1				E2			
I	J	GRASP	GRASP2K	I	J	GRASP	GRASP2K
2	22	2.993 − 01	2.444 − 01	2	11	1.852 − 01	1.742 − 01
2	23	4.006 + 00	4.866 + 00	2	12	1.656 + 00	1.691 + 00
2	24	1.189 − 02	7.164 − 01	2	15	1.702 + 01	1.313 + 01
2	26	3.194 − 01	2.629 − 01	3	8	6.833 − 01	6.686 − 01
2	27	8.176 + 00	6.828 + 00	3	10	5.317 − 01	5.253 − 01
3	4	6.537 + 02	6.601 + 02	3	13	3.847 − 01	3.621 − 01
3	5	1.503 + 02	1.505 + 02	4	14	7.596 − 01	7.437 − 01
3	16	1.093 + 01	3.300 + 01	5	13	1.207 + 00	1.199 + 00
3	17	2.078 + 00	1.155 + 01	5	14	8.823 − 01	8.658 − 01
3	18	3.613 − 01	3.387 − 01				
3	23	7.572 − 01	1.438 + 00				
3	24	4.080 − 01	2.401 − 01				
3	25	2.637 − 01	5.492 − 01				
4	5	4.290 + 00	4.087 + 00				
4	17	4.214 − 01	4.192 − 01				
4	23	1.147 − 03	1.255 − 03				
4	27	1.108 + 01	9.125 + 00				
5	16	1.040 + 00	1.498 + 00				
5	17	1.243 + 00	1.247 + 00				
5	18	2.251 + 00	7.509 − 01				
5	21	1.283 − 01	3.911 + 00				
5	24	2.047 − 01	3.525 + 00				
5	27	1.828 + 00	1.674 + 01				

GRASP: Present results with the GRASP code for 3948 level calculations; GRASP2K: Earlier results of Jönsson et al. [10] with the GRASP2K code.

Table 11. Comparison of lifetimes (τ, s) for the lowest 27 levels of Sc XII. $a \pm b \equiv a \times 10^{\pm b}$.

Index	Configuration	Level	CIV3	GRASP2K	GRASP
1	$2s^22p^6$	$^1S_0$	....	....	....
2	$2s^22p^53s$	$^3P^o_2$		4.760-05	4.462-05
3	$2s^22p^53s$	$^3P^o_1$	4.22-12	4.372-12	4.228-12
4	$2s^22p^53s$	$^3P^o_0$		1.515-03	1.530-03
5	$2s^22p^53s$	$^1P^o_1$	3.10-12	3.131-12	2.977-12
6	$2s^22p^53p$	$^3S_1$	5.11-10	5.186-10	5.161-10
7	$2s^22p^53p$	$^3D_2$	3.15-10	3.124-10	3.044-10
8	$2s^22p^53p$	$^3D_3$	2.84-10	2.879-10	2.805-10
9	$2s^22p^53p$	$^3D_1$	3.17-10	2.905-10	2.816-10
10	$2s^22p^53p$	$^3P_2$	3.27-10	2.340-10	2.276-10
11	$2s^22p^53p$	$^1P_1$	2.88-10	3.216-10	3.104-10
12	$2s^22p^53p$	$^3P_0$	2.17-10	2.184-10	2.131-10
13	$2s^22p^53p$	$^3P_1$	2.42-10	2.451-10	2.383-10
14	$2s^22p^53p$	$^1D_2$	2.67-10	2.627-10	2.559-10
15	$2s^22p^53p$	$^1S_0$	6.74-11	6.868-11	5.725-11
16	$2s^22p^53d$	$^3P^o_0$	1.29-10	1.311-10	1.287-10
17	$2s^22p^53d$	$^3P^o_1$	3.23-11	3.459-11	3.549-11
18	$2s^22p^53d$	$^3P^o_2$	1.31-10	1.334-10	1.303-10
19	$2s^22p^53d$	$^3F^o_4$	1.29-10	1.312-10	1.278-10
20	$2s^22p^53d$	$^3F^o_3$	1.20-10	1.226-10	1.190-10
21	$2s^22p^53d$	$^3F^o_2$	1.15-10	1.176-10	1.142-10
22	$2s^22p^53d$	$^3D^o_3$	1.18-10	1.207-10	1.166-10
23	$2s^22p^53d$	$^3D^o_1$	1.20-12	1.227-12	1.357-12
24	$2s^22p^53d$	$^1D^o_2$	1.15-10	1.170-10	1.131-10
25	$2s^22p^53d$	$^3D^o_2$	1.16-10	1.190-10	1.151-10
26	$2s^22p^53d$	$^1F^o_3$	1.21-10	1.234-10	1.194-10
27	$2s^22p^53d$	$^1P^o_1$	1.47-13	1.436-13	1.331-13

CIV3: Earlier results of Hibbert et al. [9] with the CIV3 code; GRASP2K: Earlier results of Jönsson et al. [10] with the GRASP code; GRASP: Present results with the GRASP code for 3948 level calculations.

Table 12. Comparison of oscillator strengths (f-values) for some transitions of Y XXX.

I	J	GRASP	DFS	I	J	GRASP	DFS
1	3	0.1347	0.120	1	39	0.0245	0.020
1	9	0.0849	0.086	1	47	0.0011	0.016
1	14	0.0035	0.010	1	53	0.5028	0.443
1	23	1.7114	0.999	1	63	4.03-6	0.003
1	27	1.7560	2.278	1	71	0.3089	0.384
1	31	0.1016	0.060	1	79	0.0463	0.025
1	33	0.3082	0.304	1	81	0.1027	0.103

GRASP: Present results with the GRASP code for 3948 level calculations; DFS: Earlier results of Zhang and Sampson [7] with the DFS code.

4. Conclusions

In this paper, energy levels have been reported for three ions, namely F-like Sc XIII and Ne-like Sc XII and Y XXX. For the calculations, the GRASP code has been adopted and CI has been included among a large number of configurations. Additional calculations have also been performed with FAC, by including even larger CI. This was necessary for accuracy assessments [24] because the existing data available for these ions are very limited. Energies have been listed for the lowest 102, 125 and 139 levels of the respective ions, although calculations have been performed for much larger ranges. This is because beyond these levels is a mixing from other configurations. However, energies for higher levels can be obtained from the author on request. On the basis of a variety of comparisons, the listed energies (in general) are assessed to be accurate to better than 1% for most levels. However, this assessment of accuracy may change if laboratory measurements in the future become available for a larger number of levels.

Radiative rates are also presented for four types of transitions, namely E1, E2, M1, and M2. Again, very limited comparisons are possible because of the paucity of other available data. However, for the majority of strong transitions, the accuracy is assessed to be $\sim$20%, which is primarily based on comparisons between the length and velocity forms. Any estimates of accuracy for particularly weak transitions with very small f-values will be unreliable. The calculated A-values have been used to determine lifetimes and have been listed for all levels. No measurements have so far been performed for any level of the three ions concerned, and theoretical results are available for only the lowest 27 levels of Sc XII, for which there are no (large) discrepancies. We hope our results listed for a large number of levels/transitions will be useful for the modelling and diagnostics of a variety of plasmas, fusion in particular.

Supplementary Materials: The data files are available online at http://www.mdpi.com/2218-2004/6/2/25/s1.

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