Cosmic gamma ray bursts – Recent developments and observations from SROSS satellites

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Amongst a dozen energetic phenomena discovered during the past quarter century, the enigma of classical gamma ray bursts (GRBs) is as great as ever, with no consensus on what causes these bursts. The once dominant galactic neutron star model of GRBs has lost its popularity to the extragalactic and cosmological models in view of COMPTON's observations. The observational efforts in tracking down these mysterious sources are at the moment truly international, with emphasis on the best localizations followed by deep searches for counterparts at other wavelengths.

COSMIC gamma ray bursts (GRBs), first reported by Klebesadel *et al.*[1], continue to remain as one of the long-standing puzzles in high energy astrophysics, after twenty-five years of their discovery. GRBs are transient, non-terrestrial phenomena occurring randomly in space and time, lasting a few ms to a few minutes and characterized by bursts of intense radiation, predominantly at gamma ray wavelengths with bulk of their emission > 100 keV. The US Vela satellites that were launched to monitor any violations of the 1963 nuclear test ban treaty, recorded these events on their gamma ray detectors as early as 1967, but the announcement of this discovery of a new class of astrophysical phenomena had to wait until 1973, when the US military allowed the information to be made public.

During the period from 1973 to 1991, over 500 bursts with fluence $> 10^{-6}$ ergs/cm^2 have been recorded by instruments mostly scintillation spectrometers flown onboard at least 20 satellites, viz. Vela, Helios 2, HEAO 1 & 2, Prognoz, ISEE-3, Solar max mission, Ginga, Apollo, etc. and inter-planetary probes like Venera 11, 12, 13, 14, Pioneer Venus orbiter, Phobos, etc. Studies on GRBs have proved difficult due to their transitory nature. The most general methodology of GRB study involves temporal and spectral studies, spatial distribution of an ensemble of bursts and other wavelength observations. Data collected on GRBs usually consist of a record of intensity variations as a function of time, over a wide energy band (Temporal profile) and energy spectra recorded at constant time intervals.

Over the years, two classes of GRBs have been recognized[2], viz. Classical GRBs, which account for the majority of bursts observed and Soft Gamma Repeaters (SGRs), three of which are known. The relation between the two, if any, is not clear. Time profiles of classical GRBs display a wide variety of shapes and durations varying from few seconds to a hundred seconds, with hard spectra (peak power at energies > 100 keV) which evolve with time. Typical rise and decay times range from 0.1 to 1 s. Classical GRBs are not known to repeat. SGRs, have nominal durations of 0.1–1 s, exhibit soft spectra with e-folding energy ~ 30 keV, which are time invariant. SGRs repeat at irregular intervals.

Although about a hundred models have been proposed to explain the origin of gamma ray bursts, none has so far been able to explain all the observations satisfactorily. The mystery shrouding soft gamma repeaters has been of late, largely resolved by multiwavelength counterpart observations. In contrast, classical GRBs have so far not been identified with any known population of objects in the universe, despite conducting deep searches to identify their counterparts at other wavelengths. As the distance to the source is as yet unknown, the total energy involved in the burst process has remained ambiguous by about 23 orders of magnitude.

With the launch of NASA's Compton Gamma Ray Observatory (CGRO) in April 1991, which carries onboard an instrument to monitor GRBs with unprecedented sensitivity, viz. the Burst and Transient Source Experiment (BATSE)[3], there has been a significant change in the quality of data and also the interpretation of the results. BATSE with its sensitivity to bursts with fluence $> 5 \times 10^{-8}$ ergs/cm^2, which is an order of magnitude superior to its predecessors, records about one burst per day and has accumulated data on about 1296 bursts till 8 June 1995 (ref. 4). Prior to Compton, there existed a wide consensus that gamma ray bursts originate due to some catastrophic event on or near the surface of a neutron star in our galaxy. The discovery by BATSE that bursters have an isotropic, but radially inhomogenous distribution in space has altered the thinking of many theorists. As CGRO observations favour a distribution greater than at least 50 kpc, the mystery on the origin of GRBs has only deepened further and at the moment it is unclear whether these are of galactic or extragalactic origin. Recent reviews on GRBs, by Hurley[5], Higdon and Lingenfelter[6] and conference proceedings edited by Fishman *et al.*[7], provide abundant information on observations, analysis and models of GRBs.

In the following sections, we review GRBs, from an observational point of view, as they were understood prior to the launch of CGRO and the highlights of results following the launch. The motivation for the Indian GRB experiments flown on the Stretched Rohini Satellite Series (SROSS-C, May 1992; SROSS-C2, May 1994) and their observations are also presented. Also discussed is the possible contribution of SROSS-C2 to the third interplanetary network of detectors currently monitoring GRBs.

Pre-CGRO era

Prior to the launch of CGRO, there existed a wide consensus that a GRB is caused by some catastrophic event near the surface of a neutron star in our galaxy. The observations suggested that most of the common classical burst sources are single, intensely magnetic neutron stars in the nearby galactic disk, and that the SGRs could be neutron stars with slightly weaker magnetic fields and possible binary companions. The circumstantial evidence which led to the galactic neutron star hypothesis was:

i) Very small source size < 1000 km, implied by rapid time variability in classical GRBs and < 60 km implied by the 0.2 ms rise time of GB790305b (ref. 8).
ii) Location of GB790305b event within the N49 supernova remnant (SNR) in the Large Magellanic Cloud (LMC) (ref. 8).
iii) Very high mean density $> 10^6$ g/cc implied as minimum density against breakup, if the 8 s period in the soft repeater GB790305b is rotational[9–11].
iv) Absorption lines between 20 and 70 keV in about 15% of classical bursts, which are attributed to cyclotron absorption in Terragauss magnetic fields[12,13]. These were further confirmed by the Japanese satellite Ginga[14] which observed bursts with two lines harmonically spaced, viz. at 20 & 40 keV.
v) Emission lines seen between 350 and 500 keV in both classes of bursts[12,13] – interpreted as gravitationally redshifted electron position annihilation radiation with neutron star redshifts of 0.1 or more[15].
vi) Failure to detect quiescent counterparts at other wavelengths within the source positional error boxes[16–22].
vii) Galactic distances implied by the black body limit derived from soft X-ray emission from GB870303 (ref. 14).

Further, the size-frequency distribution, which indirectly provides information on the radial distribution of sources, was found to follow the – 3/2 power law for bright bursts, while the distribution deviated significantly for weak bursts with a flattening at lower fluences. This flattening at low fluence was considered as an evidence of a galactic origin, with more distant sources exhibiting nonuniform spatial distribution. The angular distribution of sources was however found to be isotropic, which is not consistent with a nonuniform spatial distribution if the burst sources are members of a galactic disk or halo population[23 24].

High sensitivity balloon observations[25,26] of bursts with fluence $> 10^{-8}$ erg/cm^2 also suggested that the flattening of the size frequency distribution at low fluence was due to spatial nonuniformities and not due to selection biases. If true, the distribution of low fluence bursts would exhibit anisotropy with a concentration at low galactic latitudes. The BATSE experiment on CGRO was designed to resolve this contradiction.

The CGRO era

Compton's BATSE was designed specifically to investigate weak GRBs and localize them using its eight large 2000 cm^2 sodium iodide scintillation detectors mounted along the eight corners of the spacecraft providing an all-sky coverage. The events recorded are localized to an accuracy of a few degrees using the anisotropic response of the detectors. While this accuracy falls short of that needed to pinpoint visible counterparts, it suffices to map the burster distribution on the sky. In response to a trigger signal from BATSE, the other instruments on Compton[27], viz. Oriented Scintillation Spectroscopy Experiment (OSSE), the Compton Telescope (COMPTEL) and the Energetic Gamma Ray Experiment Telescope (EGRET) switch to a burst data collection mode, if the source occurs within their field of view. While COMPTEL can measure energy spectra of GRBs with high resolution between 0.1 and 10 MeV, it is also capable of localizing sources to about a degree. The EGRET instrument covers the broadest energy range from 20 MeV to 30 GeV. The Compton instruments have detected several unique individual events, the shortest event lasting ~ 100 μs (ref. 28), a few bright GRBs whose emission extends greater than 30 MeV (ref. 29) and two bursts from the region of SGR1900 + 14 (ref. 30). BATSE has also studied the spectra of the brighter bursts and searched for cyclotron line features[31–34]. Even though no definite evidence for lines is found, statistics do not yet support a clear inconsistency between BATSE and earlier mission results.

The most astounding result from BATSE data is that the angular distribution of GRB sources is found to be as isotropic as ever, with no concentration towards the galactic plane, or in directions of any other nearby galaxy or clusters of galaxies[35]. Figure 1 shows the spatial distribution in galactic coordinates of 1000 BATSE bursts[36]. BATSE has also detected fewer weak bursts[16] (Figure 2) than would be expected for a −3/2 power law (shown by dotted lines), implying that the source distribution is not uniform out to infinity. In other words, weaker sources are fewer than expected, indicating thereby a boundedness to the region of source confinement. As burster models have to necessarily account for these important results on spatial and intensity distributions, these results have triggered a flurry of modelling activity, with a raging controversy on the burster distance scale.

Burster models and the distance debate

Prior to the launch of Compton, there existed a wide consensus on the local heliocentric models which favour the galactic neutron star paradigm. In these models the burster population is assumed at a distance of say 100–200 pc but still within the confines of the galactic disk in the solar neighbourhood. One of the early models focused attention on the retention of a cometary cloud by a collapsing star and subsequent fall/accretion of a solid object of mass $\sim 10^{17-19}$ g onto the neutron star releasing about 10^{36-40} ergs of energy in an explosion[37,38]. Another model, viz. the thermonuclear model, first proposed by Woosley and Taam[39], received more detailed attention over the years and predicts GRBs to occur due to slow accretion of matter from a companion or from the interstellar matter, leading eventually to a helium flash when the critical density and temperature are reached. Gamma radiation is believed to be produced due to magnetic reconnection. Though these models easily explain isotropy, a decrease in the density of sources far away is not expected, as the sun does not occupy a special place in the galaxy and there is no known population of galactic objects at these distances. Considering distances larger than the galaxy's thickness, we run into the opposite problem, i.e. while the radial inhomogeneity is easily explained, an anisotropy towards the galactic plane is not seen.

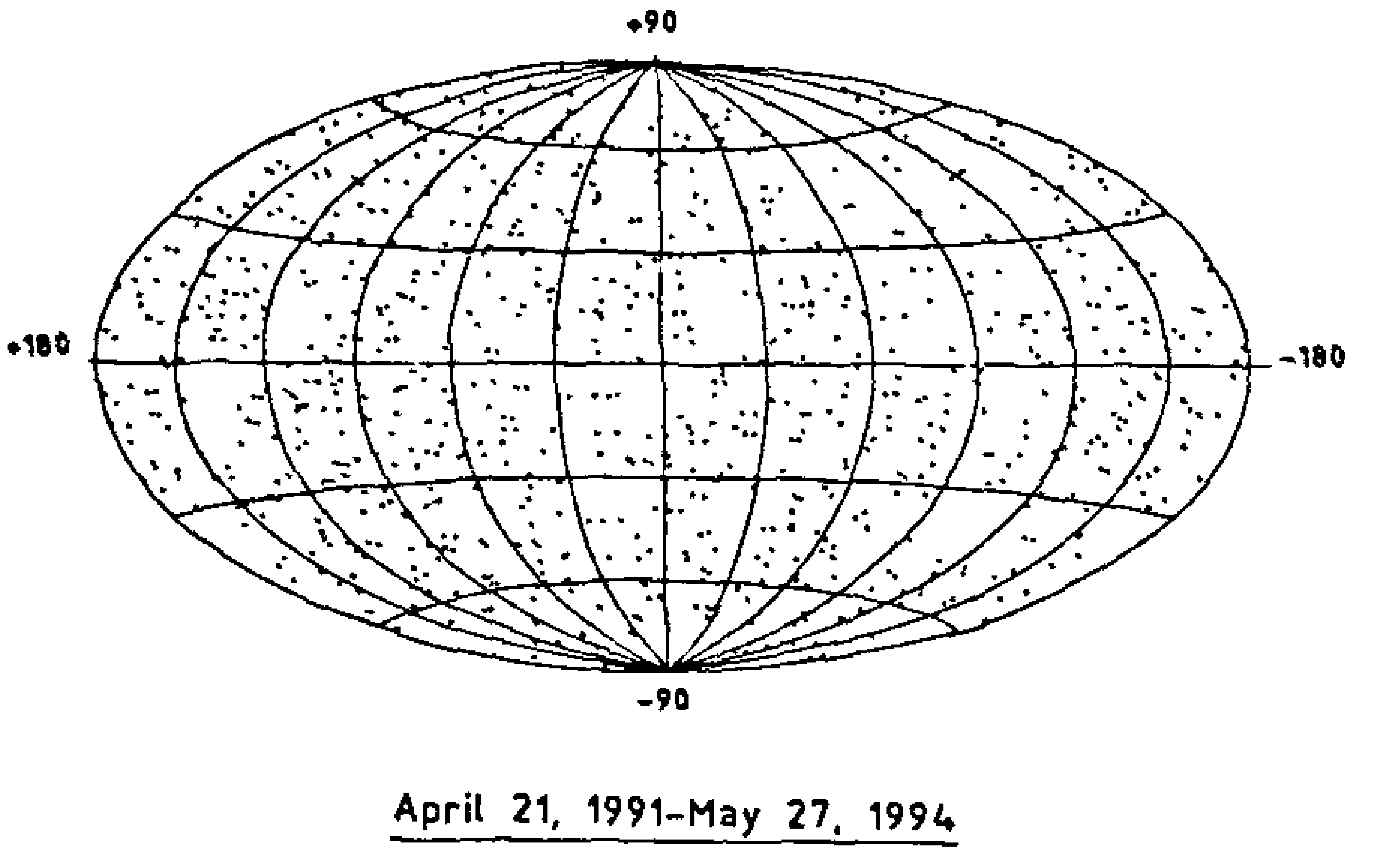

Figure 1. Spatial distribution of 1000 BATSE bursts

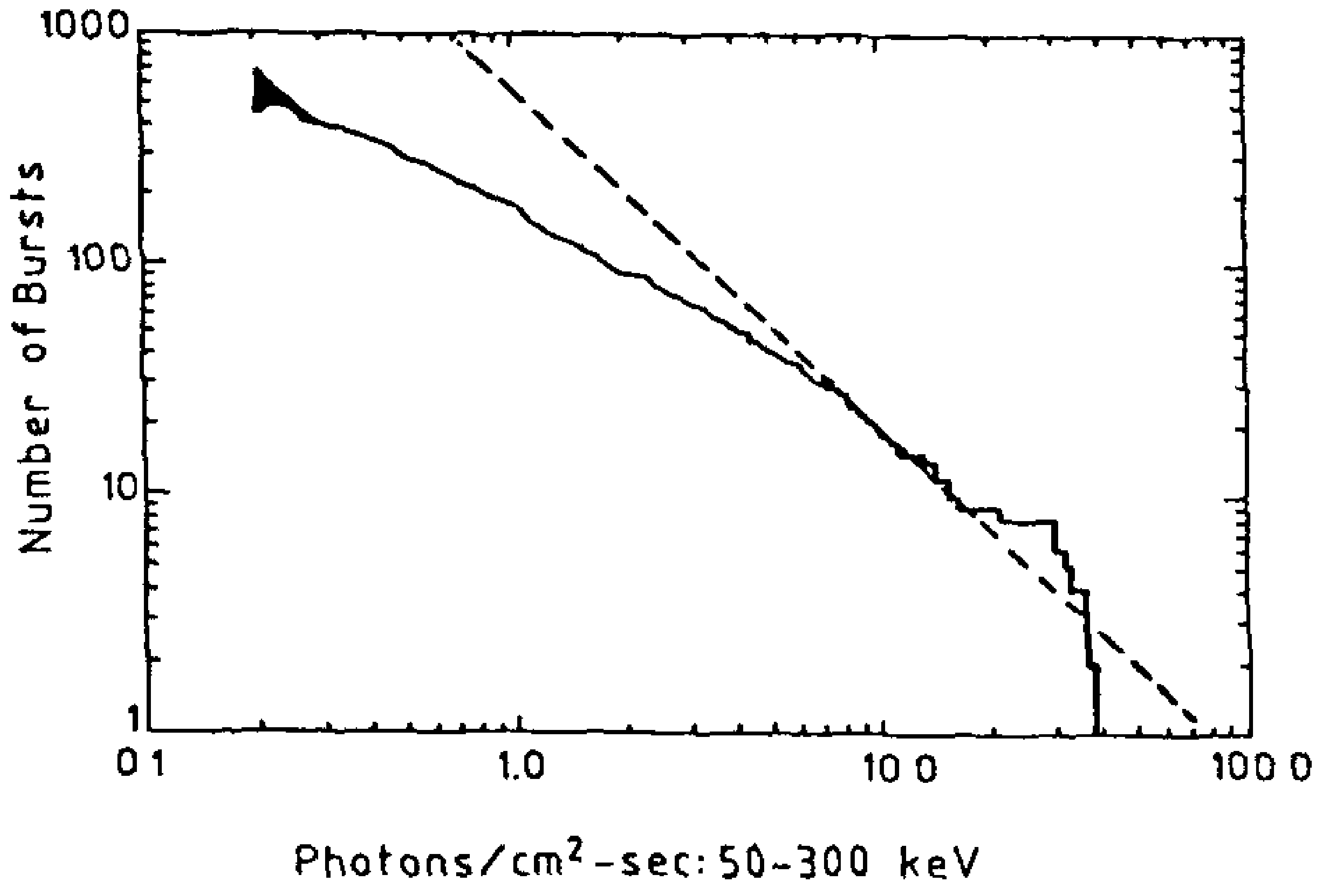

Figure 2. Integral peak flux distribution for 455 BATSE bursts

As of now, with the constraints imposed by BATSE observations on the spatial distribution of faint GRBs, the most widely accepted distance models place the GRB sources either in the outer regions of our galaxy (galactic corona models) or close to the event horizon of our universe (cosmological models). The former model postulates a source population extending about 100 kpc and centered on the galaxy such that the Sun's offset with respect to the galactic centre is negligible. While this galactic corona model explains both isotropy and radial inhomogeneity of burster distribution, the problem here is to populate a halo with neutron stars and find an explanation as to why they became active GRB sources in the halo and not when they were within the galaxy. Population II neutron stars, i.e. those formed by accretion-induced collapse of white dwarfs with birth velocities greater than 1000 km/s are believed to be shot out into the halo surrounding the galaxy[40]. Quakes on neutron stars, which produce about 10^{42} ergs of energy have been suggested as powering mechanisms[41]. As yet, there is no clear evidence supporting the existence of such a structure in the galaxy.

If the cosmological scenario is considered, isotropy follows very naturally, and the flattening of the size frequency distribution is attributed to the effects of the expansion of the Universe[42,43]. The most popular scenario for cosmological bursts involves a collision in a close binary consisting of a black hole and a neutron star or two neutron stars. The orbit of a binary neutron star, particularly those with tight orbits like binary pulsars, decays due to emission of gravitational radiation and eventually coalesces and merges releasing 5×10^{53} ergs mostly as a neutrino burst or as gravitational energy. For GRBs to be detectable at cosmological distances, only a fraction as small as 10^{-3} of this energy is required to be converted to gamma rays. Such events are estimated to occur in the universe at a rate of 10^{-6} per year per galaxy which is comparable to the GRO burst detection rate. It also follows that other cosmological effects like time dilation, redshift and gravitational lensing should be observable in the weak bursts. Recently an announcement of time dilation in faint BATSE bursts by a factor of 2 has been adduced as evidence[44] for the cosmological distance scale.

At the moment, the mystery of gamma bursters has only deepened and is awaiting some observations or theoretical developments that would settle the dispute on the distance scale. Since neither the location of GRB sources nor their repetition rates are known, pre-planned observations in other wavebands are not feasible. Quiescent counterparts of bursters have been sought both in survey catalogues of unusual objects which might lie in any of the burst error boxes and in deep observations of the more precise error boxes in various wave bands. Since detectors more sensitive than the BATSE are unlikely to be built and flown for some more time to come, the only hope on resolving the GRB puzzle may be pinned down to observations of GRB counterparts at other wavelengths.

Search for counterparts

The success of any search for counterparts relies heavily on the ultimate size of the error box that can be achieved. GRBs being infrequent phenomena, require omnidirectional detectors, as accurate pointing from a single detector is not practicable. The location of the source is determined post facto either by using the angular dependence of several detectors[24,45] or by the triangulation technique[23] using the time difference in the arrival of the signal between two spacecrafts. While the single satellite method is capable of localizing sources with accuracies of only a few degrees, the latter method is necessary to reduce the size of the error box to several tens of arcmin or better so as to facilitate observations at other wavelengths.

The searches for counterparts of the SGRs have been too successful and it now appears certain that SGRs may be related to young magnetized neutron stars in supernova remnants. SGR0526-66, which emitted the historic burst of 5 March 1979, was detected by about ten spacecrafts and triangulation has yielded an association with the SNR N49 in the LMC. This source has burst sixteen times over the years and a faint X-ray source consistent in position with the GRB error box has been detected by ROSAT[46]. The other two repeaters, viz. SGR1806-20 and SGR1900 + 14, have been observed by CGRO to turn ON again[47]. SGR1806-20 has produced 100 bursts irregularly spaced in time between 1979 and 1985 and 6 bursts in 1993 (ref. 47). A galactic SNR G10.0 – 0.3 (ref. 48) and an X-ray source AX1805.7-2025 (ref. 49) have been associated with the SGR1806-20. Simultaneous X-ray and gamma ray bursts have also been observed by the Japanese ASCA satellite and CGRO[50]. SGR1900 + 14 has burst 6 times during 1979–1993 and is probably associated with the galactic SNR G42.8 + 0.6, although its location lies just outside the remnant[51]. At this time, as the nature of classical GRBS is not known, this provides a strong encouragement for counterpart searches as most GRB models require some counterparts to be detectable at some wavelength on some timescale.

Search for counterparts of classical GRBs during the quiescent states, inside GRB errorboxes, has been attempted in all wavebands[52], viz. soft X-ray, ultraviolet, optical, infrared and radio bands. About a dozen optical transient images of astrophysical origin found on archival plates[53] are reported, but their relation to GRBs is unclear. While flaring and fading phase (few hours to few days) searches have technologically limited the observations to X-ray, optical and radio wavebands, until recently searches on timescales shorter than a day were not possible. With BATSE and COMPTEL positions available within a few hours of the burst[54], and the response time of interplanetary networks being about one day[55], fading phase observations are expected to be more fruitful in the near future.

The Interplanetary Network (IPN)

The success of counterpart search depends on the best localizations possible with a network of interplanetary satellites, by the triangulation technique. At the present time, USA's Compton Gamma Ray Observatory and India's SROSS-C2 satellite in near earth orbits, Russia's GRANAT[56] in a highly eccentric orbit around the earth, the international Ulysses probe[57] in a solar polar orbit and the international WIND[58] spacecraft heading for placement at the first Lagrangian point of the Earth–Sun system carry instruments that form the third interplanetary network of GRB monitors.

The GRANAT spacecraft carries three experiments which can record gamma rays, viz. SIGMA – a coded mask telescope; PHEBUS – six Bismuth Germanate scintillation detectors (each 48 cm^2 area) for recording and localizing GRBs; and WATCH – a wide angle telescope. The PHEBUS experiment records bursts of the $> 10^{6}$ ergs/cm^2 fluence class and the other two experiments compliment this data with their imaging capability. The WIND spacecraft carries two experiments which are capable of recording data on GRBs, viz. the Konus-W gamma ray spectrometer which has two identical sodium iodide detectors (120 cm^2 area) and the Germanium Transient gamma ray spectrometer (TGRS) which is meant for conducting high resolution spectral measurements on GRBs with a sensitivity to fluence greater than a few times 10^{-7} ergs/cm^2.

The hard X-ray detectors on Ulysses consist of two hemispherical thallium-doped caesium iodide shells (40 cm^2 area) each coupled to a photomultiplier tube, providing essentially an all-sky view. The instrument is sensitive to bursts with fluence $> 10^{-6}$ ergs/cm^2 and records a burst once every 3–4 days. The solar probe is presently over the North polar region (June 1995) of the sun.

The SROSS satellites

The Indian SROSS-C and SROSS-C2 satellites carrying the GRB experiment were launched on 20 May 1992 and 4 May 1994 respectively, with the objective of

a) monitoring GRBs in the energy range 20 keV–3 MeV with a sensitivity to bursts of fluence $> 5 \times 10^{-6}$ ergs/cm^2
b) monitor intensity variations with high time resolution (2 ms)
c) search for periodicities in the time histories
d) determine the evolution of the energy spectra with time and
e) search for cyclotron absorption features in the 20–100 keV energy range and look for possible redshifted annihilation radiation line in the 400–500 keV range.

Both satellites were of octagonal prismoidal shape, carrying the payload on their topdeck, and launched into a 45° inclination low earth orbit. The spin stabilized spacecrafts have their spin axis parallel to the detector view axis and along the negative orbit normal (Figure 3), thereby permitting a half sky coverage less the region (~ 34%) occulted by the earth due to low earth orbit. In addition, due to the high inclination orbit, about 30% of observing time is lost owing to passage through the South Atlantic Anomaly (SAA) and high latitude regions.

The experiment on SROSS-C had two sodium doped caesium iodide scintillation detectors, a main (44 cm^2 area), a redundant (11 cm^2 area) and a common microprocessor (CDP1802) based electronics[59,60]. The SROSS-C2 payload (Figure 4), however, carries only the main detector with its associated electronics[61]. The SROSS-C payload could record data on only one event between consecutive readouts, while the payload onboard memory in the case of SROSS-C2 is enhanced to hold the data on seven events. This feature has enhanced the duty cycle of the payload from ~ 40% in SROSS-C to about 70% in SROSS-C2.

SROSS GRBs

The experiment flown on SROSS-C worked very satisfactorily during the entire mission life of 55 days. It recorded 3 candidate GRB events, which were however not detected by GRB detectors onboard other satellites in the interplanetary space and hence remained unconfirmed[62].

SROSS-C2, which has been in orbit for the past one year, has a life expectancy of about 5 years. After the placement of the satellite in its final orbit (620 × 430 km) on 10 July 1994, the GRB payload has been operating flawlessly in meeting with its design goals. The payload records an average of one or two events every month and has recorded 15 events up to 30 May 1995. Table 1 gives the shortlisted SROSS-C2 GRB events. Of these, 13 events have so far been confirmed for detection onboard other GRB monitors. In order to confirm an event, the structure, rise time, decay time, duration and intensity of the temporal profiles recorded on different satellites have to agree with one another within their errors of measurement. Events coincident with Ulysses, BATSE of CGRO, and WIND are marked U, B and W respectively.

The event detected by SROSS-C2 on 6 January 1995 was not detected by Ulysses, presumably due to its faintness. For the event in orbit 1448, Ulysses had a rate increase in its detector, but not a trigger. As the Sun was within the field of view of the detector, this event could possibly be of solar origin. The sensitivity of the SROSS–GRB payload, implies a detection rate of ~ 18 events per year and is consistent with the observations. A mosaic of a few events is shown in

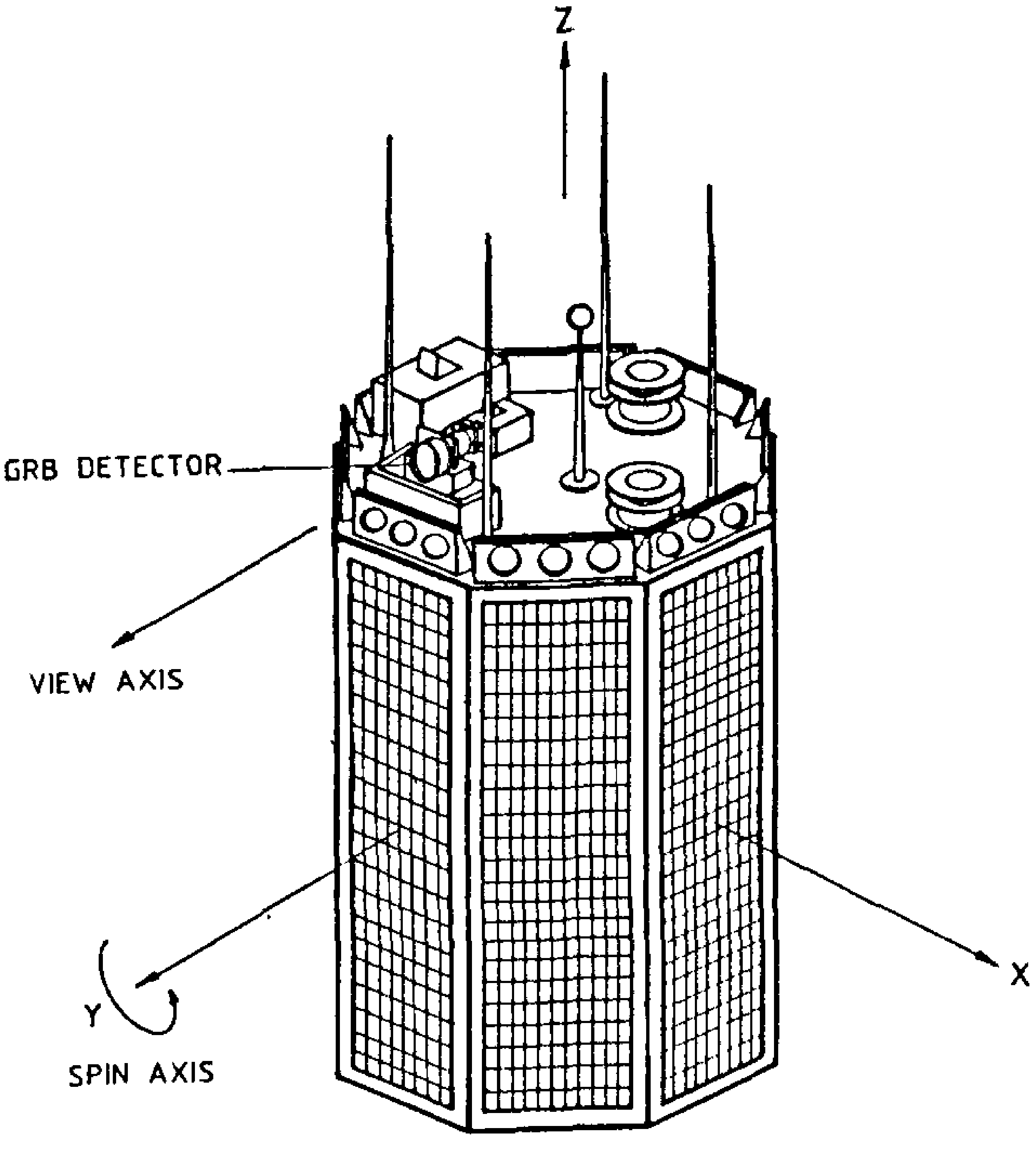

Figure 3. SROSS-C2 with GRB detector mounted on the top deck.

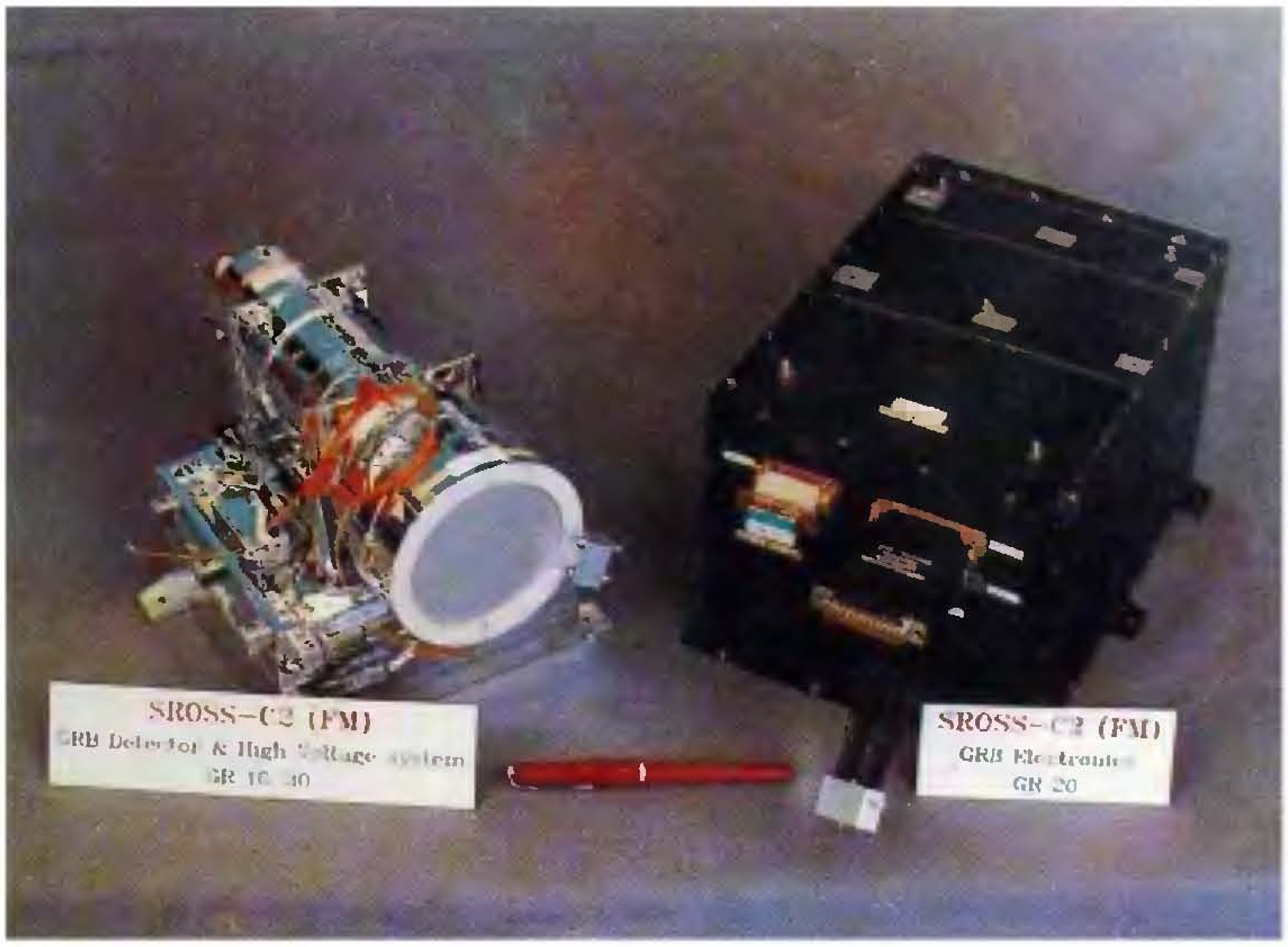

Figure 4. The gamma ray burst payload.

Table 1. SROSS-C2 GRB events

Event orbit	Event date	Time (UT) h m s	Event confirmed by
1126	19 Jul 94	06 00 05 614	U
1296	30 Jul 94	11 01 30 658	U, B
1448	09 Aug 94	11 52 31 791	—
1650	22 Aug 94	20 23 19 878	U
2095	21 Sep 94	05 08 19.368	U, B
2234	30 Sep 94	10 02 06.008	U
2492	17 Oct 94	10 19 59 748	U
3099	26 Nov 94	12 23 05.244	U, B, W
3305	10 Dec 94	03 10 53 906	U, W
3719	06 Jan 95	10 39 57 330	—
4138	03 Feb 95	02 21 29 308	U
4259	11 Feb 95	02 24 57 626	U, B
5101	07 Apr 95	15 15 31.312	U
5497	03 May 95	18 36 10 626	U, B
5622	12 May 95	00 16 48 280	U, W

U, Ulysses, B, BATSE, W, WIND.

Figure 5. As seen from the table, all confirmed events are coincident with Ulysses, while only 5 are coincident with CGRO. The reason probably could be attributed to the fact that Ulysses being a solar probe in an orbit which is presently out of the ecliptic plane has essentially an all-sky view, while both SROSS-C2 and CGRO being low-earth orbiting satellites undergo earth occultation of sky and loss of observing time due to passage through high latitudes and the SAA.

Most events last typically few tens of seconds, with the exception of two, one on 22 August 1994 and the other on 11 February 1995, which lasted about 400 ms and 128 ms respectively. The weakest burst detected by the payload so far has a fluence of about 3×10^{-6} ergs/cm^2. The normal characteristics of GRBs, viz. bimodal distribution of burst durations i.e. < 2 s and > 2 s; spectral hardness and intensity correlation etc. are all seen in our data base, albeit its small size. Analysis of all the confirmed events is being reported elsewhere.

Tracking down the GRB sources

With a few of the recent counterpart observations on Soft Gamma Repeaters being successful, it appears that these might be a separate population of sources, probably related to young pulsars in supernova remnants. However, the nature and origin of 'classical' GRBs remains one of the most compelling astrophysical problems, in view of the isotropy results of BATSE on CGRO. The solution to this problem, at the moment, demands observations that will settle the burster distance scale unambiguously. It is thus evident that a reliable statistical analysis and identification of the phenomenon with a definite class of astronomical objects requires the knowledge of as many source locations as accurately as possible. With each IPN, the triangulation baselines have grown progressively longer and have reached around 6 AU, the longest ever, when Ulysses was close to Jupiter, permitting localizations as fine as 0.1 arcmin^2. Although greater than 2000 GRBs have been recorded till date, about a 1000 or so are localized to a few degrees and only a dozen to few arcmin^2 (ref. 63).

The future efforts on tracking down the sources rely

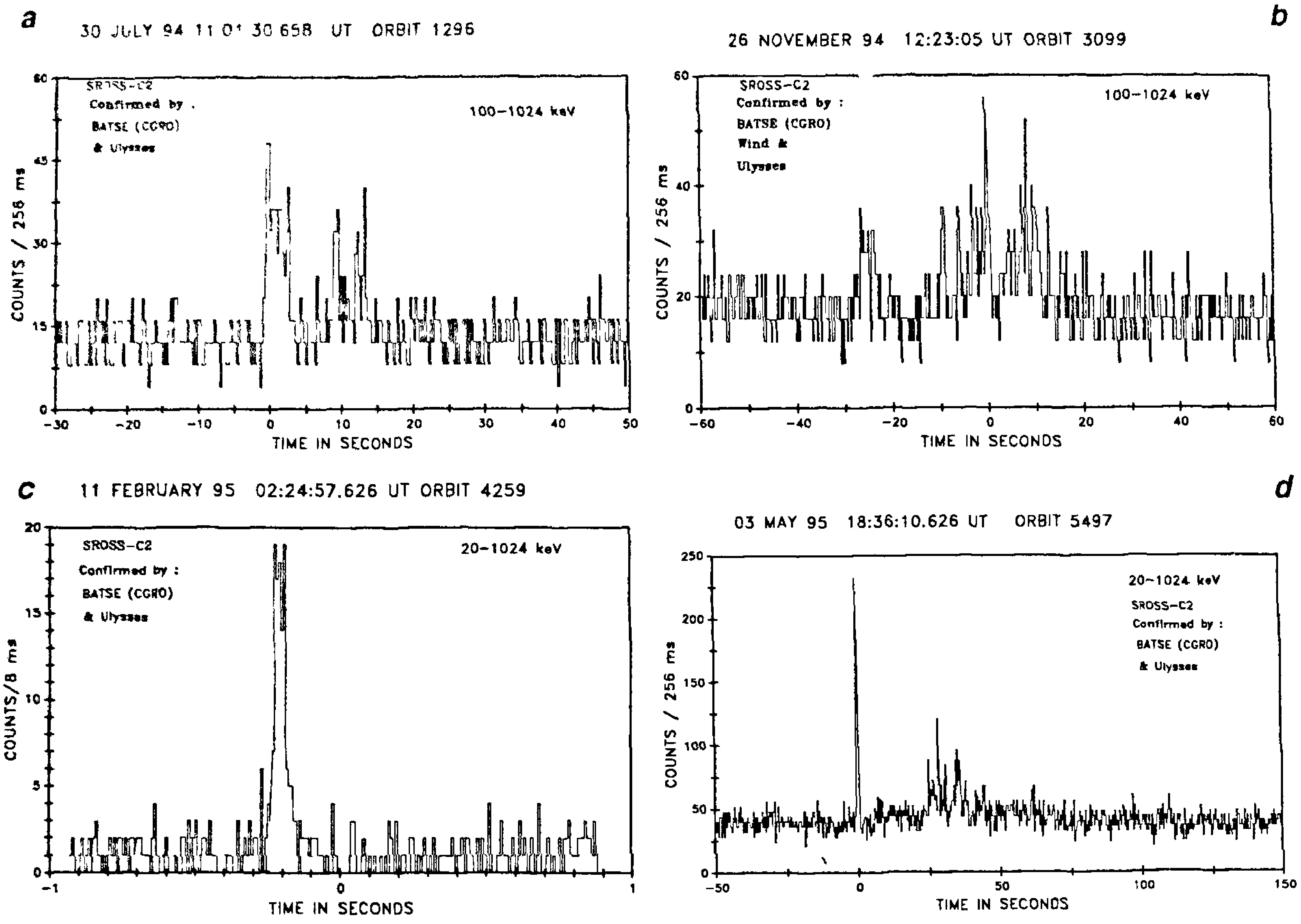

Figure 5. A few events detected by SROSS-C2

on rapid response campaigns between CGRO and fast slewing ground-based radio and optical telescopes. Multi-wavelength (gamma, X-ray and ultraviolet) observations are planned onboard the high energy transient experiment[64] (HETE) scheduled for launch in late 1995. HETE intends to localize GRBs in the UV band to arcsecond accuracy, although it is not proven that optical flashes accompany GRBs.

Since all near-earth spacecrafts undergo earth occultation, complete sky coverage at all times requires more than one instrument in near-earth space. The GRB experiment on SROSS-C2 is expected to fulfil this function and complement data obtained by CGRO and GRANAT in near-earth space. While the SROSS-C2 payload is not designed to participate in any rapid response campaign, or conduct multiwavelength observations, it is expected to detect about 80–90 bursts during its 5-year life time, of which most are likely to be coincident with Ulysses and WIND. Since Ulysses, WIND and SROSS-C2 do not independently possess the ability to localize GRBs, the class of events, coincident between these three spacecrafts, but not necessarily coincident with CGRO, would form a complement to the CGRO–Ulysses–WIND data base. We hope to record at least a dozen such events. With this, SROSS-C2 would play an important role in the international efforts of tracking down the GRB sources.

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Quantum Monte Carlo techniques: Chemical applications

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Quantum Monte Carlo (QMC) methods are stochastic simulation methods for quantum many-body systems. Here we provide an overview of QMC methods designed for simulation of atomic and molecular systems, and discuss main ideas behind the variational, diffusion and path integral QMC methods. We also review application of these techniques to some problems of interest in chemistry.

> The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are (thus) completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be solvable. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

SINCE P. A. M. Dirac wrote the above lines in 1929 (ref. 1), both the range of approximate quantum mechanical methods, and the notion of what constitutes 'too much computation' have undergone dramatic changes.

Over the past few decades, chemists have come to understand the interactions and dynamics of small molecules and clusters very well. Both theory and experiment can, for instance, provide a very accurate