Electronic Supplementary Information

The Zintl Ion $[As_7]^{2-}$: An Example of an Electron-Deficient As_x Radical Anion

Sukhendu Mandal[a], Ran Liu[a], Arthur C. Reber[b], Meichun Qian[b], Héctor M. Saavedra[a], Xianglin Ke[c], Peter Schiffer[c], Saikat Sen[d], Paul S. Weiss*[a,c,e], Shiv N. Khanna*[b] and Ayusman Sen*[a]

[a]*Department of Chemistry, The Pennsylvania State University, University Park, PA 16802, USA Fax: 814-863-5319, E-mail: asen@psu.edu*

[b]*Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, USA Fax: 804-828-7073,E-mail: snkhanna@vcu.edu*

[c]*Department of Physics ,The Pennsylvania State University, University Park, PA 16802, USA*

[d]*Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560012, India.*

[e]Current address: *California NanoSystems Institute, Department of Chemistry & Biochemistry, University of California, Los Angeles, CA 90095, USA, Fax: 310-267-4918, E-mail: psw@cnsi.ucla.edu*

Experimental Section

General Methods. All of the reagents used were commercially available and used without further purification. 4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane (2,2,2-crypt), anhydrous ethylenediamine (en) (99.5%, purified by redistillation, packed under Ar), lithium perchlorate and lithium tetrafluoroborate were purchased from Aldrich. Potassium (99.95%, ampouled under Argon), was purchased from Alfa Aesar. Tetrahydrofuran (THF) was dried by passing through an activated alumina column followed by deoxygenation by passing over a copper catalyst. All glassware (oven dried), reactants, and solvents were stored in a glove box filled with argon.

All manipulations were performed in an argon-filled glove box. The detailed synthetic procedures of the precursors K_3As_7 is summarized below:

Precursor K_3As_7: The precursors, K_3As_7 were synthesized by mixing of As (~700 mg) with a preheated mixture of K (~120 mg) and en (3 ml) in a scintillation vial [K and en mixture was stirred at 50 °C for 1 h to dissolve K partially in en to produce a blue solution]. This mixture was continuously stirred for 30 min at 50 °C followed by the addition of 3 ml of en and the mixture was stirred overnight at room temperature. The red suspension was filtered through an Acrodisc premium 25-mm syringe filter with GxF/0.2 μm pores (syringe filter) and the resulting dark red solution was used for further reactions. Note: As and K metals did not completely dissolve.

Single Crystal Structure Determination

X-Ray diffraction data were collected at 120 K on a Bruker APEX diffractometer with a CCD area detector equipped with an X-stream 2000 cryo-system low-temperature device. A suitable crystal for compound **1** was carefully selected under a polarizing microscope and

mounted on a loop using N-Paratone oil and quickly placed under the nitrogen flow of the cryo-stream. The X-ray generator was operated at 50 kV and 32 mA using Mo Kα (λ = 0.71073 Å) radiation. Data were collected with a ω scan width of 0.3°. A total of 600, 430, 235 and 50 frames were collected in four different settings of φ (0°, 90°, 180°, 270°) keeping the sample-to-detector distance fixed at 5.8 cm and the detector position (2θ) fixed at -25°. Pertinent experimental details of the structure determination of compound **1** are presented in Table S1.

The data were reduced using SAINTPLUS[S1] and an empirical absorption correction was applied using the SADABS[S2] program. The structure was solved by direct methods using SHELXS97 and refinement against F^2 was carried out using the SHELXTL V6.1 package of programs.[S3] Each of four following arsenic atoms in the $[As_7]^{2-}$ cluster were disordered over two positions with occupancies as given below (the disorder was modeled using the PART instruction):

Atom	**Site occupancy**	**Atom**	**Site occupancy**
As3A	0.83005	As3B	0.16995
As4A	0.82511	As4B	0.17489
As6A	0.79608	As6B	0.20392
As7A	0.73755	As7B	0.26245

For the final refinement, the hydrogen atoms were placed in geometrically ideal positions and refined using the riding mode. The last cycles of the refinement included atomic positions, anisotropic thermal parameters for all atoms other than hydrogen, and isotropic thermal parameters for all the hydrogen atoms.

Other Experiments

The yield of the reaction is 85% and single crystals are monophasic in nature. We have checked cell parameters for several crystals which match the crystal data of **1**. We have used powders derived from single crystals for magnetic, EPR and the solid state band-gap measurements. The crystals were washed with ethylenediamine and dried in vacuum in glove box and finely ground to the powder form prior to the measurements. Cyclic voltammetry experiment was carried out with solid K_3As_7 compound.

Powder X-ray Diffraction: Powder XRD patterns were taken with a Rigaku (RU-200) X-ray generator equipped with a Guinier camera (G670 from Huber Diffraktiontechnik GmbH and Co. KG) using monochromatized CuKα (λ = 1.5418 Å) radiation. The finely powdered single crystals were placed on Milar film (on a holder) in the argon filled glove box. The sample was covered with another film. The holder with sample was tightened with a ring. The junction of the holder and ring was covered with high vacuum grease. The XRD pattern of compound **1** is consistent with the XRD pattern simulated from the single crystal structure (Figure S3), suggesting that the powder consists of pure **1**. Data was collected on Milar film to check the background noise.

Magnetic Measurement: Magnetic studies were carried out using a SQUID magnetometer (Quantum Design Inc., USA) over the temperature range 1.8 to 160 K at a magnetic field of 100 Oe. The inherent sensitivity of the SQUID set up allows for very accurate (up to 10^{-7} emu = 10^{-7} erg/G) measurements of the sample's magnetization to be made. The powder samples (ground single crystal) of **1** were loaded in a glass capillary and sealed with high vacuum grease in the argon filled glove box. The capillary was then placed inside of a standard plastic drink straw. Measurements were made on an empty glass capillary to insure that the background from the sample mounting was negligible.

Electron Paramagnetic Resonance: EPR measurements were performed on Elexsys 500 machine operating at 9.3897 GHz frequency. The powder samples (ground single crystal) of **1** were loaded in the EPR tube and sealed with septum and high vacuum grease in the argon filled glove box. The spectra of **1** were recorded between 5 and 100 K using liquid He cryostat. Measurements were made on an empty EPR tube to insure that the background from the sample mounting was negligible.

Cyclic Voltametry: Cyclic voltametry studies were performed on a SP-150 Bio Logic potentiostat using a Pt-stripe working electrode Pt-stripe counter electrode and Ag/AgCl reference electrode (in 3 M KCl). DMF was used as solvent. 0.1 M lithium tetrafluoroborate was used as supporting electrolyte. Cyclic voltammograms were run at scan rate of 100 mV/s from -0.8 V to 0.8 V at room temperature under Ar atmosphere in a glove box.

Solid-State Band Gap Measurements: Diffuse reflectance spectra were collected at room temperature using a Perkin Elmer Lambda 950 UV-Vis-NIR spectrophotometer, equipped with a Harrick Praying Mantis diffuse reflectance accessory. A photomultiplier tube was used for detection in the 320-860.5 nm range, while a lead sulfide detector was used for the 860.5-2300 nm range. The spectra were collected from 320-2300 nm, with 1.0 nm resolution and integration times of 0.64 s. A dry and finely ground magnesium oxide (MgO) powder was used as a reflectance reference material. Prior to any measurements, single crystals of compound **1** were finely ground and diluted with MgO to 30% by weight.

For a crystalline solid with a band gap (E_{bg}), the frequency dependence (ν) of the absorption coefficient (κ) can be approximated as:

$$\kappa(\nu) = \frac{B_T(h\nu - E_{bg})^n}{h\nu},$$

where B_T is a constant derived from the square of the averaged dipolar momentum matrix element, and n is equal to 0.5 and 2 for *direct* and *indirect* band gap transitions, respectively. The formula for indirect band gap was used in this case.

Theoretical calculations: The electronic structures of compound, **1** were calculated by the VASP code[S4] based on the density-functional theory, which uses a plane-wave basis and PAW pseuopotentials[S5] to describe the electron-ion interaction. The Perdew-Burke-Ernzerhof (PBE) formalism[S6] was used for exchange and correlation potentials and energies. Brillouin zone integrations were carried out on a Monkhorst-Pack[S7] grid of 4x2x2 k-points, using the tetrahedral method. The kinetic energy cut-off of 300 eV is used for the plane wave basis. The atomic positions were optimized until the forces were less than 10 meV/Å. The calculations were spin unrestricted, and ferromagnetic, antiferromagnetic, and nonmagnetic ground states were considered.

The electronic orbitals and eigenstates of the free clusters were determined by using a linear combination of Gaussian orbitals molecular orbital approach within a density functional theory (DFT) formalism. For all atoms, we employed the DFT optimized DZVP basis set.[S8] The actual calculations were based on the deMon2K set of codes (see ref. S9 and references therein). The exchange-correlation potential was calculated using the orbital charge density. All the structures were fully optimized in redundant coordinates without symmetry constraints, and spin unrestricted calculations were performed for As_7^{2-}.[S9] Optical spectra were calculated using TD-DFT using the ADF code,[S10] and the solvent was simulated by using the COSMO method.[S11]

References

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Table S1. Crystal data and structure refinement parameters for compound $[K(2,2,2\text{-crypt})]_2[As_7].THF$, **1**.

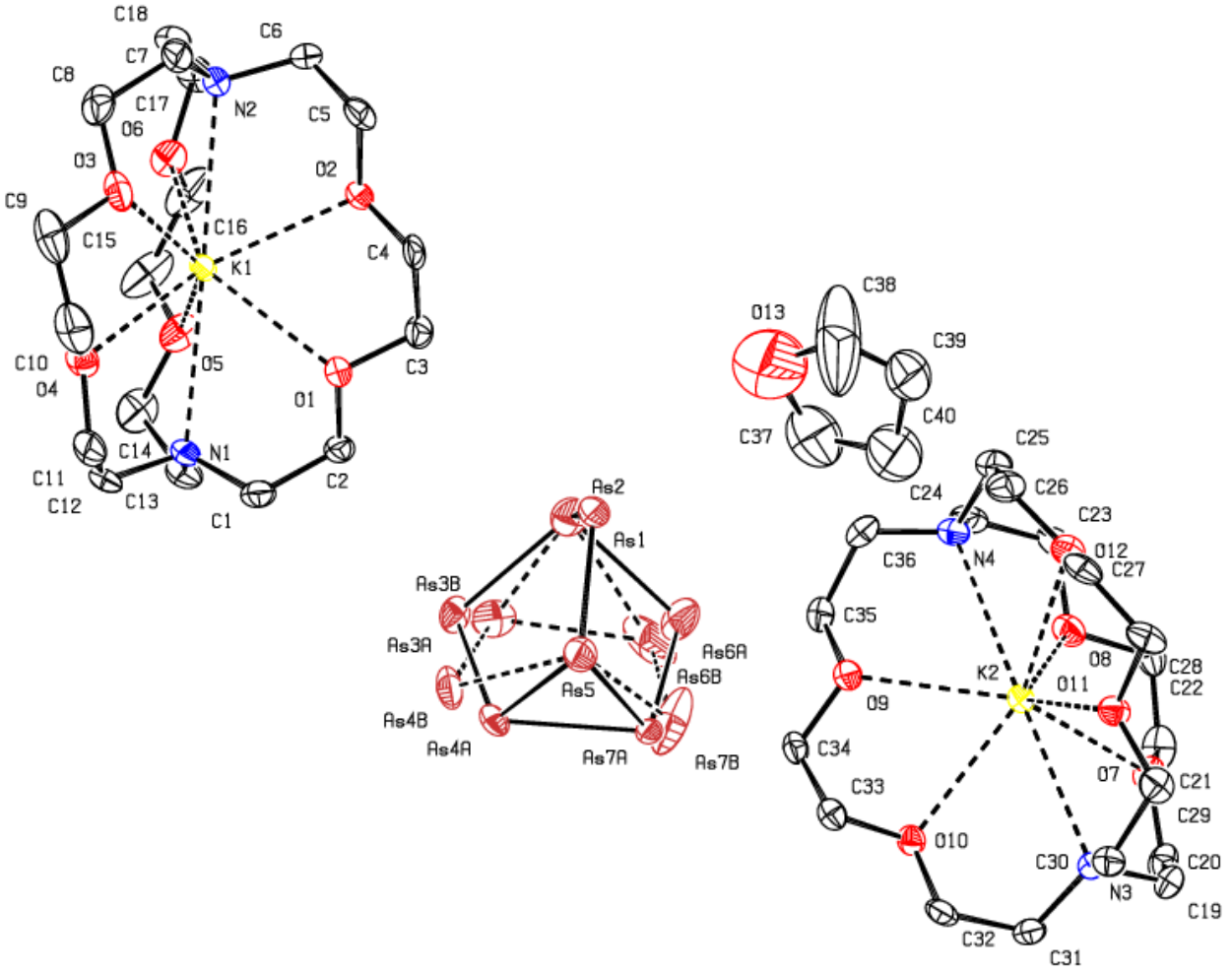
Empirical formula	$C_{40}H_{80}As_7K_2N_4O_{13}$
Formula weight	1427.72
Crystal system	Triclinic
Space group	*P*-1 (No. 2)
a (Å)	10.862(3)
b (Å)	12.933(4)
c (Å)	21.592(6)
α (deg)	102.376(5)
β (deg)	96.120(6)
γ (deg)	100.964(5)
Volume ($Å^3$)	2873.9(13)
Z	2
Size (mm)	0.18 x 0.12 x 0.05
T (K)	120(2)
ρ_{calc} (g cm^{-3})	1.650
μ (mm^{-1})	4.221
θ range (deg)	0.98 to 26.00
Reflections collected	23518
Unique reflections	11211
Number of parameters	635
Goodness of fit (S)	0.984
Final R indices [I>2sigma(I)]	$R_1 = 0.0534$, $wR_2 = 0.1163$
R (all data)	$R_1 = 0.0817$, $wR_2 = 0.1280$
Largest diff. peak and hole (e.$Å^{-3}$)	2.230 and -1.567

$R_1 = \Sigma|| F_o | - | F_c || / \Sigma | F_o |$; $wR_2 = \{\Sigma [w (F_o^2 - F_c^2)]/\Sigma [w (F_o^2)^2]\}^{1/2}$.

$w = 1/[\rho^2(F_o)^2+(aP)^2+bP]$. $P = [\max (F_o, O)+2(F_c)^2]/3$, where a = 0.0536 and b = 0.0000 for compound **1**.

Table S2. Selected As – As bond distances in compound $[K(2,2,2\text{-crypt})]_2[As_7].THF$, **1**.

Bond	**Distance (Å)**
As1 – As2	2.3723(10)
As1 – As5	2.3398(11)
As3A – As2	2.4195(16)
As3A – As4A	2.3466(17)
As3B – As2	2.1673(63)
As3B – As4B	2.3570(16)
As4A – As5	2.4117(12)
As4A – As7A	2.4715(35)
As4B – As5	2.7397(56)
As6A – As2	2.4470(34)
As6A – As7A	2.4076(45)
As6B – As2	2.5074(11)
As6B – As3B	2.5081(25)
As6B – As7B	2.3252(27)
As7A – As5	2.4409(29)
As7B – As5	2.5751(12)
Av. (As – As)	**2.4272**



(a)

Fig. S1a. ORTEP diagram of the of $[K(2,2,2\text{-crypt})]_2[As_7].THF$ **1**, with the atom numbering scheme for the asymmetric unit. Displacement ellipsoids have been drawn at 50% probability level. The hydrogen atoms have been omitted for clarity. The dotted lines in the $[K(2,2,2\text{-crypt})]^+$ cation indicate dative bonds of the cryptand to the K^+ ion, whereas those in the disordered $[As_7]^{2-}$ cluster indicate the As–As bonds involving As3B, As4B, As6B and As7B.

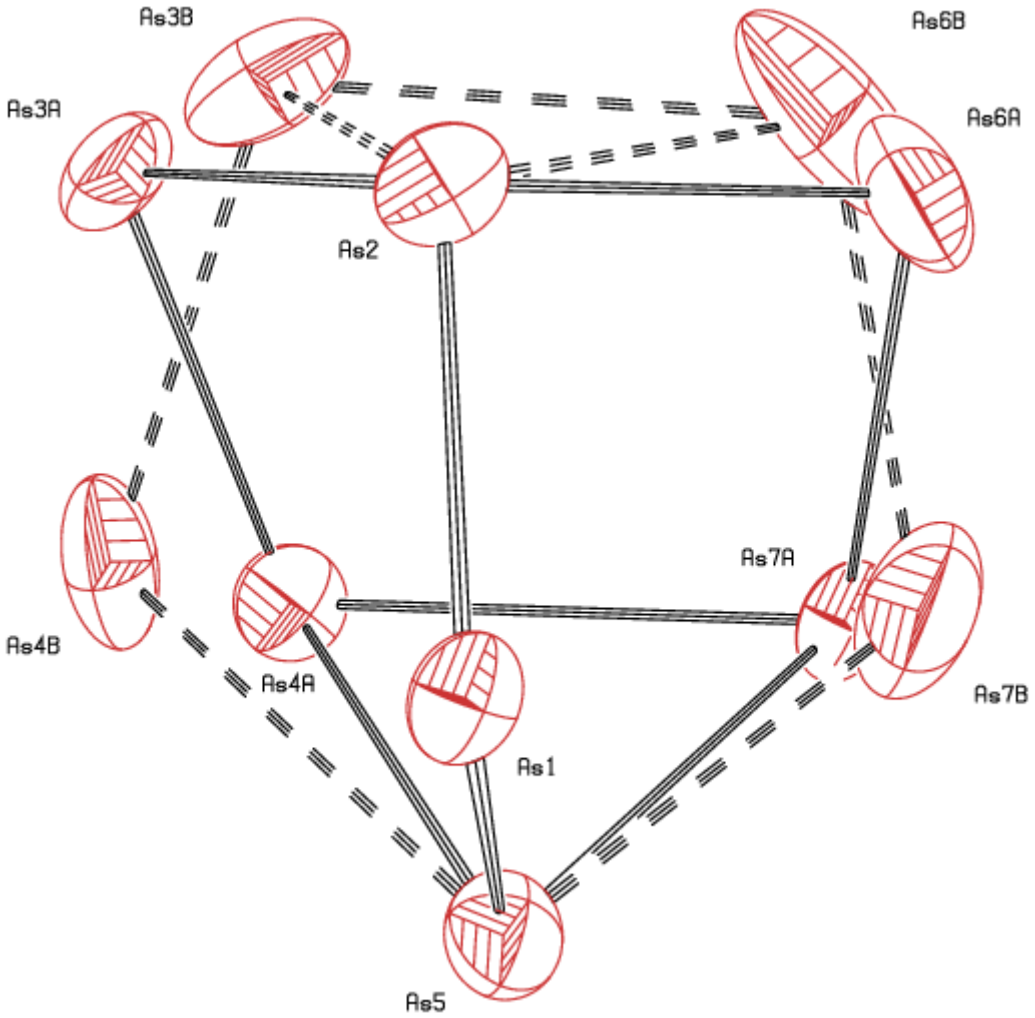


Fig. S1b. A detailed view of the As–As bonds in the disordered $[As_7]^{2-}$ cluster

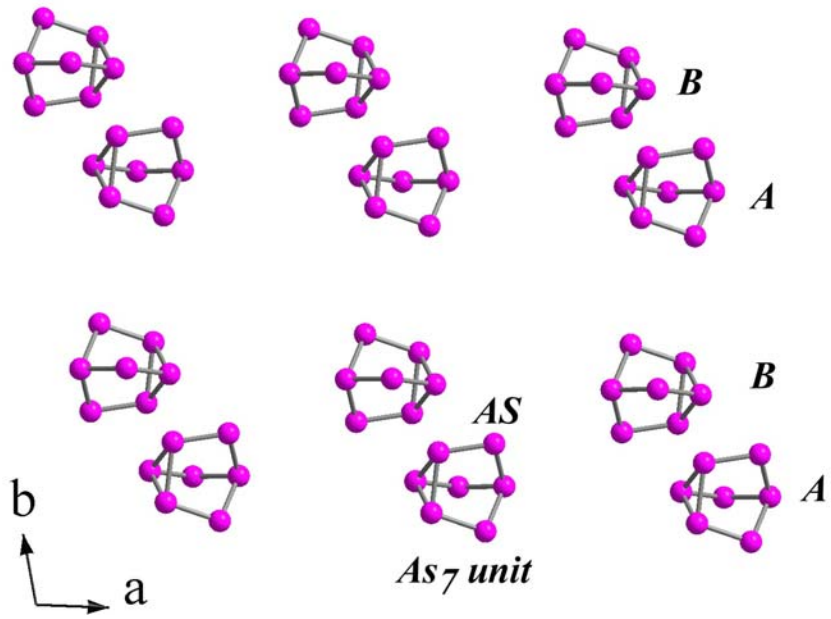


Fig. S2. The ABAB arrangement of the As_7 cluster of $[K(2,2,2\text{-crypt})]_2[As_7].THF$, **1** in the *ab* plane.

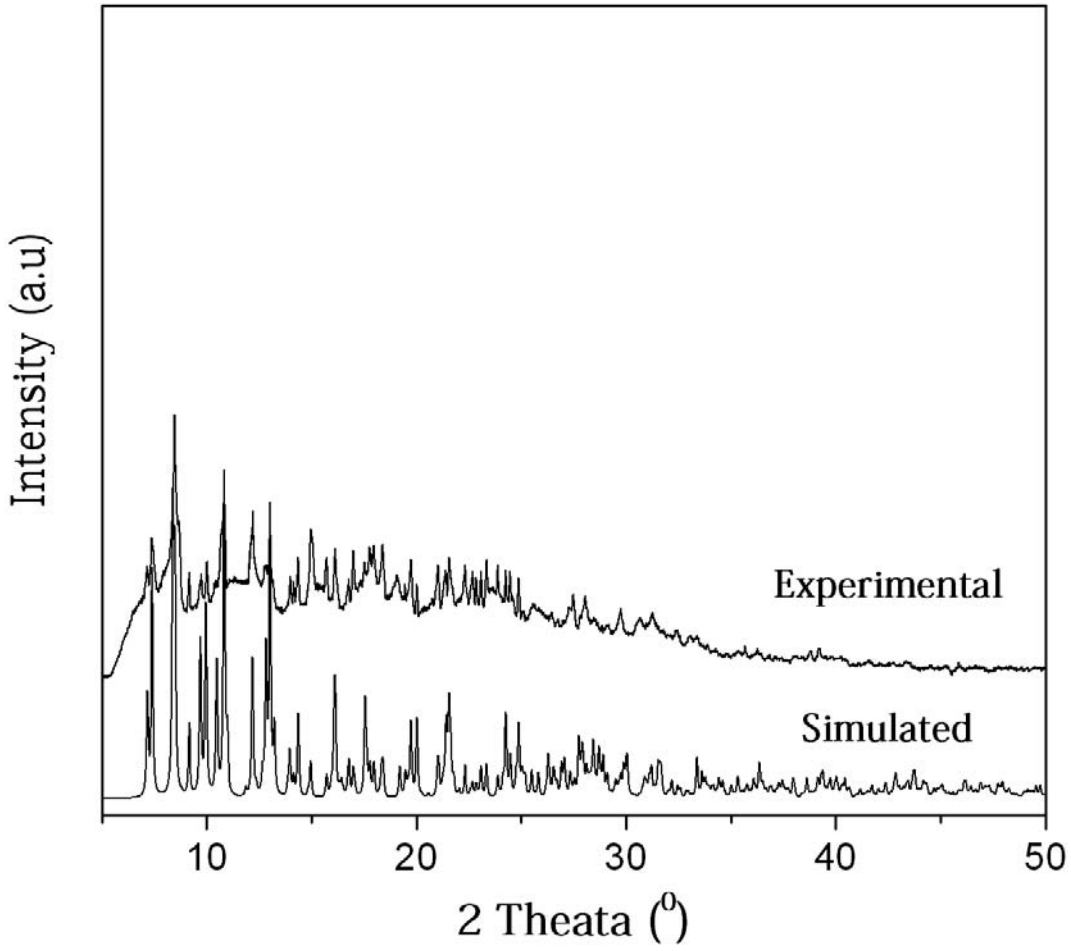


Fig. S3. Simulated and experimental powder pattern of compound **1**.

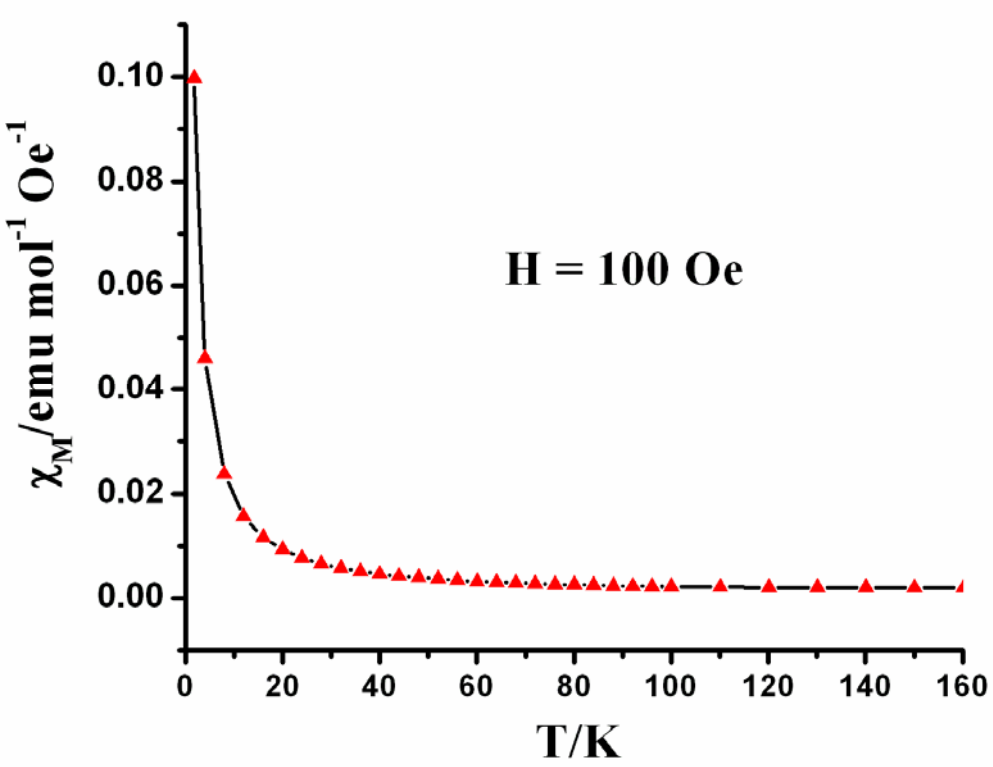


Fig. S4. χ_M vs. T data of **1** at 100 Oe.

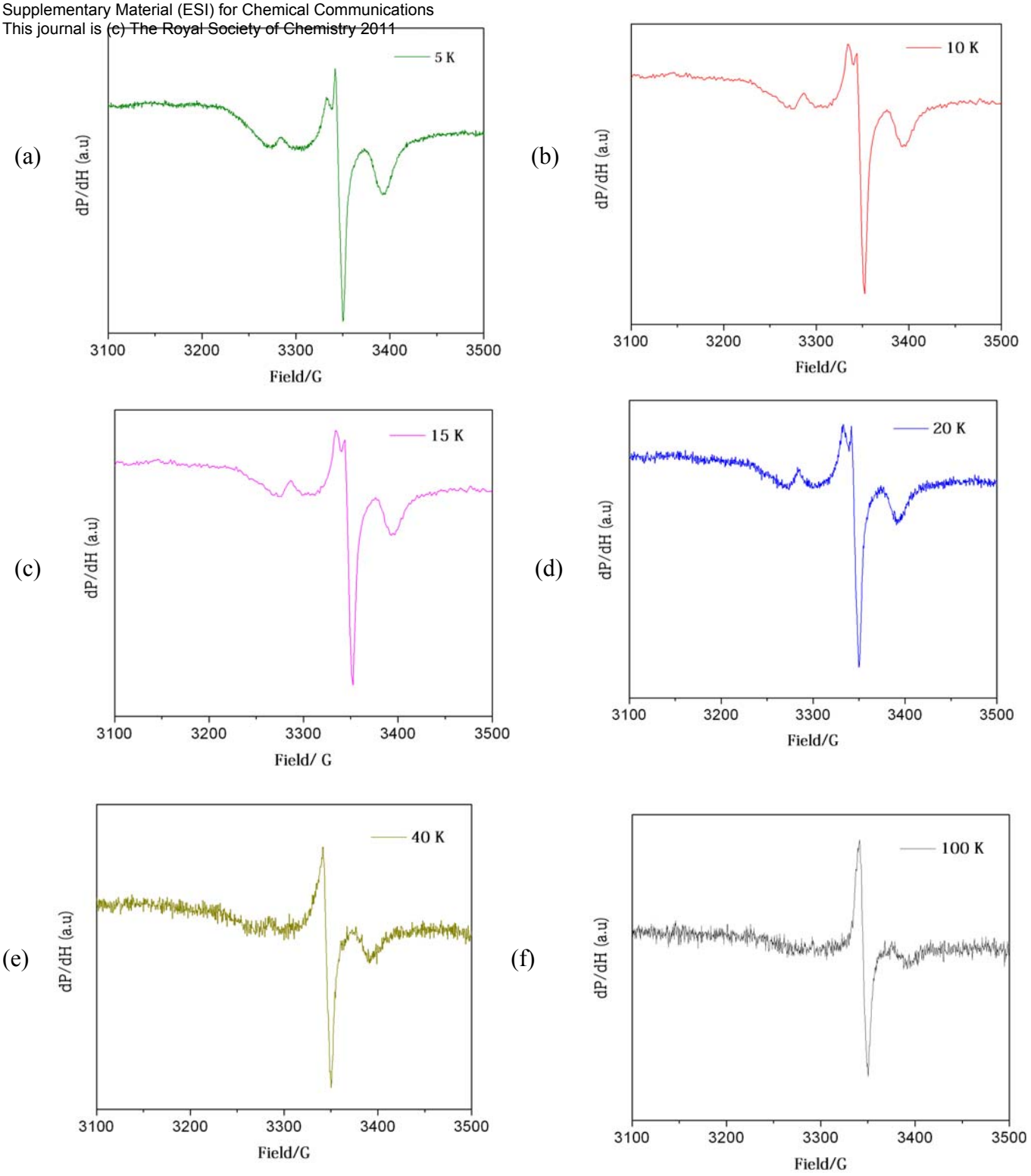


Fig. S5. EPR data of **1** at different temperature ranging from 5 – 100 K (a – f).

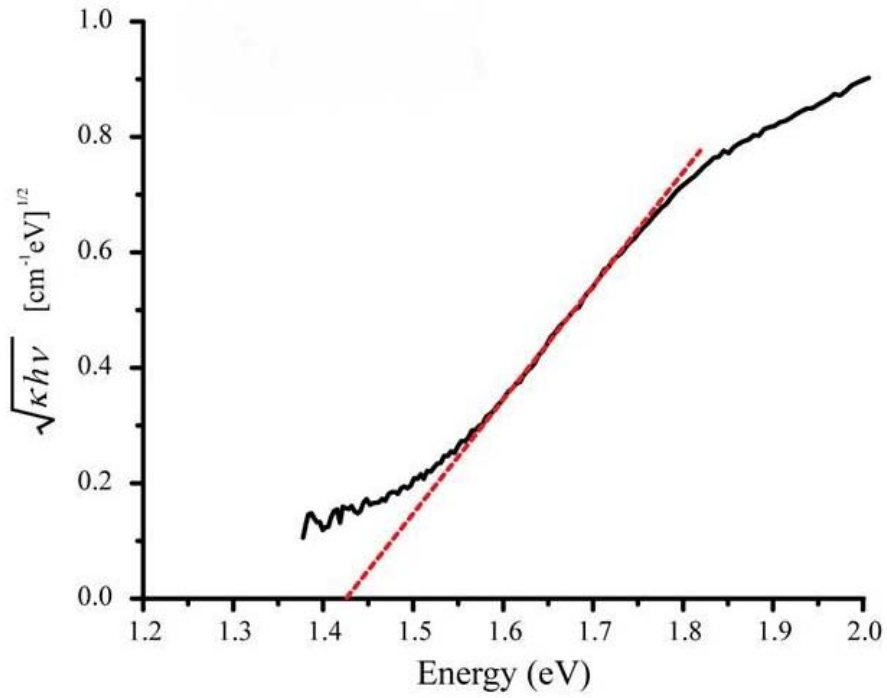


Fig. S6. Tauc plot showing the band gap determined from the optical absorption spectra of compound $[K(2,2,2\text{-crypt})]_2[As_7].THF$, **1**.

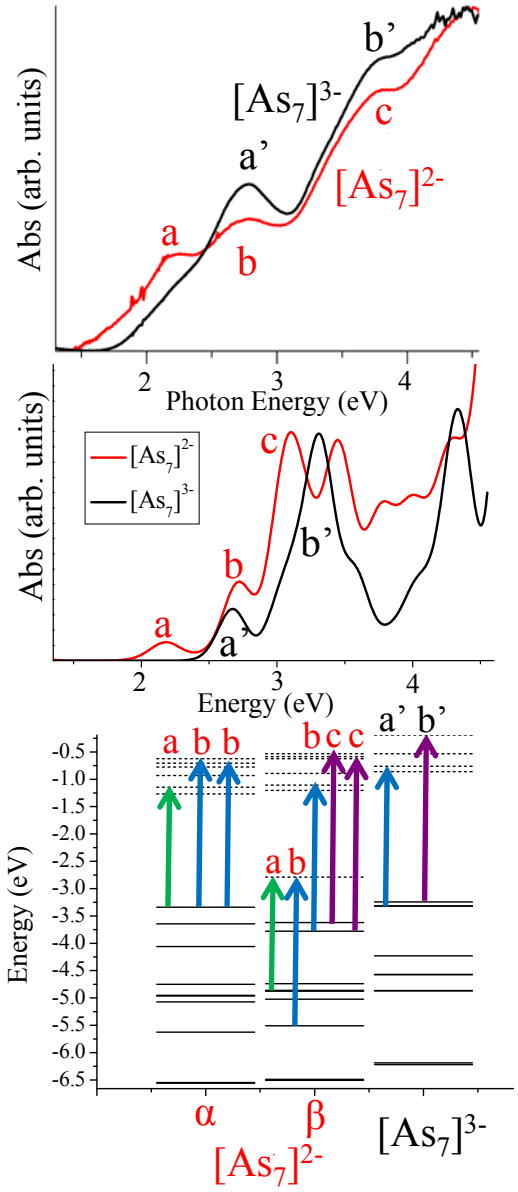


Fig. S7. Experimental UV-Vis spectra of $[As_7]^{2-}$ and $[As_7]^{3-}$. Calculated UV-Vis spectra of $[As_7]^{2-}$ and $[As_7]^{3-}$, and the primary transition which produce the spectra. Red indicates the observed peak associated with the transition, red labels are for $[As_7]^{2-}$ black labels are for $[As_7]^{3-}$.

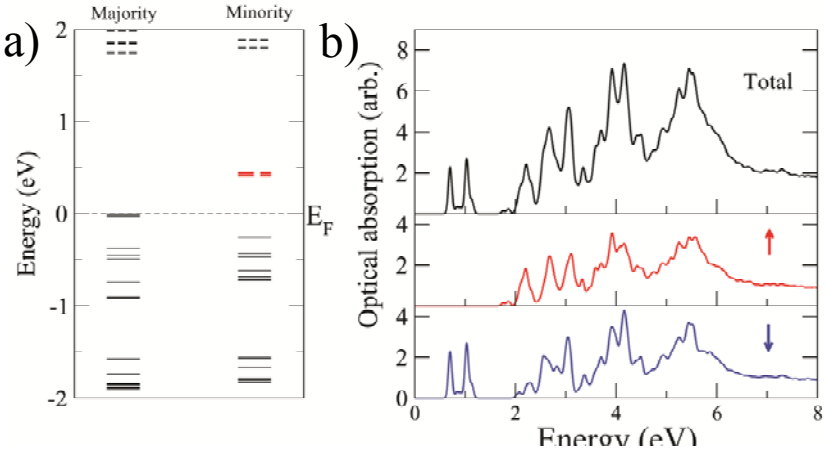


Fig. S8. a) Calculated one-electron levels at the Gamma point of the [K-crypt]$_2$[As$_7$] material and b) the calculated absorption spectra.

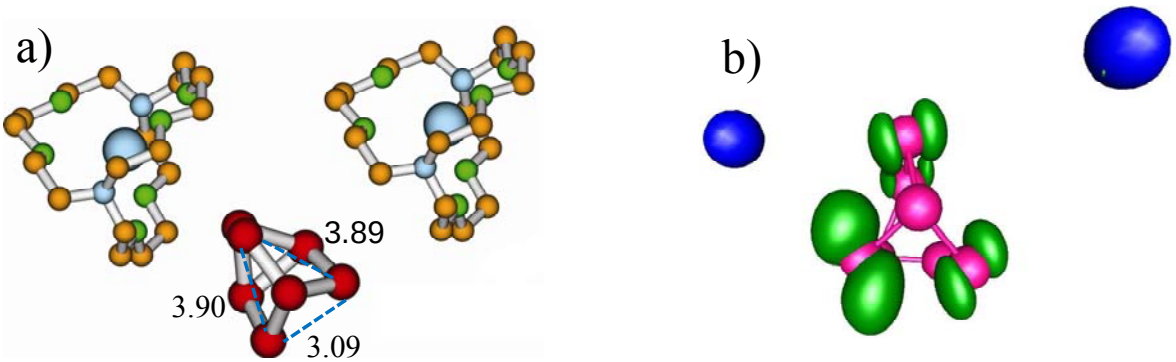


Fig. S9. a) Calculated geometries and b) electron spin density (in green) of the $[K\text{-crypt}]_2[As_7]$ in a ferromagnetic (FM) solid state. Bond lengths are in angstroms (Å).

XYZ Coordinates from Theoretical Calculations.

(1). Ferromagnetic arrangement (Figure S8), all coordinates in angstroms.
Total energy = -59.26833 Hartree
Unit Cell Parameters:

a = 10.890
b = 12.948
c = 21.563
alpha = 102.283
beta = 96.156
gamma = 100.940

Space Group Number = 2
Space Group Symbol = P-1

Cell Volume = 2882.138 Z=2

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As 0.83496257 4.42306625 6.21063164
As -1.46868944 3.90914163 6.30510429
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As 9.16865548 1.47940715 5.80065517
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As -3.05033396 6.11531082 15.01940821
As -2.55912810 4.38021491 16.80690482
As 6.27594572 4.67221893 18.07447634
As 5.68596633 6.80849590 15.90926836
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C 0.47322613 8.45984891 0.78492605
C 3.35374510 8.51416391 5.15906499
C 2.46790318 7.47992555 4.51327993
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C 6.10946267 10.49781274 3.65941773

C 5.15434553 10.01905783 4.73533072
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C 4.26634255 4.59492245 1.48462541
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C	-1.19159064	5.73831763	10.12860903
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C	3.76703280	7.17801976	10.51606472
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O	5.68521304	-3.86380697	19.88103614
O	0.93516368	7.85973014	18.41922322
O	5.32841228	4.83122547	0.55037127
O	0.83235834	-2.04553031	20.80919786
O	-0.90919914	-2.61879629	12.81649176

O	1.19818092	-1.51601178	11.16691188
O	-1.44052658	0.69697362	15.06160278
O	1.02969437	1.67249737	14.03648973
O	7.38743105	0.50506345	11.20166479
O	-1.20353028	2.08556796	10.38976011
O	7.02863664	10.21179652	8.00343759
O	4.92102069	9.10952254	9.65189509
O	7.56241487	6.89794518	5.75594746
O	5.09348914	5.92194990	6.78114838
O	-1.26660033	7.08817325	9.61837761
O	7.32345918	5.50838014	10.42959840
O	0.98352645	5.91253847	13.42288720
O	5.13734902	1.68356656	7.39293071
H	2.73533804	9.34501660	5.57369758
H	3.91874204	8.03321146	5.98960461
H	3.09318589	6.72070580	3.98537830
H	1.88853337	6.92687867	5.28911815
H	0.16762490	6.58018837	3.70651790
H	1.33522053	6.43211566	2.37599212
H	-1.08275785	7.20336668	1.76441893
H	-0.69497455	8.72211460	2.61403130
H	-2.46770119	1.93901195	20.01423326
H	1.04488270	6.44681216	0.34550331
H	1.58660716	3.84348707	18.66095134
H	2.01602903	2.09638664	18.69285909
H	7.36254730	11.68424066	1.69560681
H	5.93853954	12.06105658	0.69162546
H	6.90106248	11.13020829	4.13749782
H	6.61259215	9.60583455	3.23936123
H	5.74261236	9.57707827	5.57226340
H	4.56052625	10.85894613	5.16447780
H	6.26258626	1.52960677	2.60401581
H	6.61893589	0.57953419	1.12033673
H	-1.48882340	11.24193059	0.13421506
H	-1.21097681	10.44898030	1.74834857
H	0.25537604	11.77323266	3.00917067
H	1.89589083	0.29728361	1.99443336
H	4.14749741	1.03103440	1.10517100
H	3.87444974	1.31806029	2.85652947
H	8.40953508	0.55897890	2.95204317
H	7.22971211	-0.17044303	4.05012263
H	4.98806514	5.02973420	20.65085186
H	6.87870182	9.17679736	1.28339484
H	3.33498659	2.45199750	20.79391911
H	3.96366621	3.37298995	19.36696022
H	-0.34333914	1.65933733	18.89494970

H -0.70337348 3.40824317 18.94635682
H -3.65688736 3.92489070 20.49337548
H -2.25053378 4.59072823 19.99431803
H 3.38773817 -1.75146238 15.24598235
H 2.20488949 -0.43928616 14.82968505
H 3.02983779 0.87231360 16.83510989
H 4.23430525 0.66678437 15.53109579
H 5.95675780 1.01181438 17.11338660
H 4.78818701 1.16153042 18.44277090
H 7.20465053 0.38898196 19.05747292
H 6.81736971 -1.12964638 18.20767115
H 8.58433359 5.65464982 0.80646650
H 5.07233476 1.14498080 20.47371718
H 4.52181191 3.74476854 2.15887183
H 4.10078071 5.49421244 2.12452992
H -1.24398516 -4.09178924 19.11775482
H 0.17813285 -4.46880031 20.12455878
H -0.77805179 -3.53776540 16.67725308
H -0.49184764 -2.01342588 17.57607319
H 0.38171503 -1.98404631 15.24475324
H 1.56376875 -3.26550232 15.65407154
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H -0.49869321 7.01602006 19.69915461
H 7.60798132 -3.64943292 20.68794430
H 7.33262737 -2.85611420 19.07359600
H 5.86516205 -4.17859642 17.81020892
H 4.22503670 7.29707667 18.82432050
H 1.97344987 6.56269581 19.71353071
H 2.24650239 6.27574375 17.96219368
H -2.28808761 7.03351807 17.86577263
H -1.10770840 7.76281490 16.76822340
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H -0.76017212 -1.58426062 19.53148099
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H -0.94653528 1.83040096 16.74862485
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H 6.81740388 0.59709815 14.65664892
H 5.50579651 -1.36592266 13.27827824
H 6.65268852 -1.86899053 12.00273826
H 7.00847171 -3.13039333 14.31406300
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H 1.94753026 2.81112666 9.48104138
H 0.96532536 3.40265191 10.85456759
H 5.33474861 0.20374553 11.49318446
H 6.16660649 1.07406157 12.81411015
H 3.28198443 2.66881032 11.75207925
H 3.09661450 1.12347436 12.60843278
H 2.53835859 3.13607758 13.94713253
H 1.10244778 3.45269218 12.92465636
H 3.14212750 -1.59212834 10.37914893
H 2.99144097 -0.82489053 11.99348096
H 1.71881924 -2.60701120 12.87942245
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H 6.40672977 8.39783861 13.36680872
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H -1.25404066 5.02248103 9.27777267
H -0.21812726 5.57565167 10.64480636
H 6.40180610 4.60610731 12.10422388
H 6.12883635 6.35353185 11.94022865
H 2.74965064 6.81873711 10.81927780
H 4.32929393 7.33656595 11.45615244
H 9.09901715 -1.60779258 9.86794611
H 8.52825221 -0.68974761 8.42876475
H 6.45819861 4.49572942 6.06648934
H 5.03761775 4.80594410 4.99928697
H 5.90552449 7.09692125 4.47510069
H 7.06696572 5.76818546 4.06681319
H -2.00605675 7.02918254 4.14370005
H 8.05790402 8.55972813 4.58112994
H -0.40536671 8.49945503 5.24239577

H	-0.69552843	6.99668985	6.16294920
H	0.61524743	8.95949039	7.54231574
H	-0.53198205	9.46210940	8.81772453
H	-0.88886572	10.72412849	6.50661236
H	-2.41307770	10.12527896	5.82507390
H	4.17223659	4.78223279	11.33635954
H	5.15630013	4.19138680	9.96383069
H	0.78619332	7.38917416	9.32709820
H	-0.04575206	6.51920562	8.00597184
H	2.83977995	4.92407488	9.06343793
H	3.02550923	6.46963561	8.20760912
H	3.58604334	4.45717745	6.86943057
H	5.02137371	4.14162319	7.89298319
H	2.97649643	9.18494040	10.43831652
H	3.12848805	8.41841120	8.82377652
H	4.40072783	10.20044629	7.93926992
H	6.60997537	-1.65406077	9.50675071
H	-0.28586405	-0.80506493	7.45543321
H	0.40682550	-1.80384660	8.78785447
H	1.32845213	9.18930270	13.78699785
H	2.62424707	8.15848796	13.11465693
H	2.95386997	7.36211835	15.29706008
H	1.37986587	7.98605453	15.87115238
H	0.28693700	5.94711441	15.40277646
H	1.92458550	5.22296103	15.13738888
H	-0.38494080	7.49820651	13.31157040
H	0.70244944	7.26262909	11.88657432
H	4.79602740	-1.59342090	7.02859449
H	3.49820463	-0.56577191	7.70151341
H	3.16707975	0.23396674	5.52116929
H	4.73992830	-0.39053429	4.94449120
H	5.83573344	1.64762616	5.41346227
H	4.19777446	2.37255426	5.67741664
H	6.50643792	0.09859596	7.50681119
H	5.41712358	0.33403968	8.93028541

(2). Free Cluster: K_2As_7

As	0.00000	0.00000	0.00000
As	0.00000	0.00000	2.43088
K	3.26472	0.00000	0.61260
As	0.54819	2.33724	-0.41541
K	-2.91865	1.44082	0.64311
As	2.14591	3.12224	1.32797
As	-0.53732	3.75149	1.32789
As	-0.83258	2.22281	3.24982
As	1.73560	1.61695	3.24715