Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Actinide sulfides in the gas phase: Experimental and theoretical studies of the thermochemistry of AnS (An = Ac, Th, Pa, U, Np, Pu, Am and Cm)

Cláudia C. L. Pereira,[a] Colin J. Marsden,*[b] Joaquim Marçalo*[a] and John K. Gibson[c]

[a] *Unidade de Ciências Químicas e Radiofarmacêuticas, Instituto Tecnológico e Nuclear, 2686-953 Sacavém, Portugal*

[b] *Laboratoire de Chimie et Physique Quantiques, UMR 5626, IRSAMC, Université Paul Sabatier, 31062 Toulouse Cedex 9, France*

[c] *Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

Supplementary information

Table S1 Reaction products and kinetics for the reactions of AnS^+ with 1,3-butadiene and isoprene[a]

Reactant ion	**C_4H_6**	***k*/k_{COL} [*k*]**	**C_5H_8**	***k*/k_{COL} [*k*]**
ThS^+	$ThSC_2H_2^+$ (45)	0.40 [0.41]	$ThSC_2H_2^+$ (15)	0.43 [0.45]
	$ThSC_4H_4^+$ (40)		$ThSC_3H_4^+$ (30)	
	$ThSC_4H_6^+$ (15)		$ThSC_5H_5^+$ (5)	
			$ThSC_5H_6^+$ (40)	
			$ThSC_5H_8^+$ (10)	
US^+	$USC_2H_2^+$	0.22 [0.23]	$USC_2H_2^+$ (35)	0.31 [0.32]
			$USC_3H_4^+$ (30)	
			$USC_5H_6^+$ (30)	
			$USC_5H_8^+$ (5)	
NpS^+	$NpSC_2H_2^+$	0.19 [0.20]	$NpSC_2H_2^+$ (40)	0.21 [0.22]
			$NpSC_3H_4^+$ (35)	
			$NpSC_5H_6^+$ (25)	
PuS^+	$PuSC_2H_2^+$	0.20 [0.21]	$PuSC_2H_2^+$ (40)	0.42 [0.43]
			$PuSC_3H_4^+$ (25)	
			$PuSC_5H_6^+$ (25)	
			$PuSC_5H_8^+$ (10)	
AmS^+	$AmSC_2H_2^+$	0.25 [0.26]	$AmSC_2H_2^+$ (40)	0.30 [0.30]
			$AmSC_3H_4^+$ (35)	
			$AmSC_5H_6^+$ (25)	
CmS^+	$CmSC_2H_2^+$	0.40 [0.41]	$CmSC_2H_2^+$ (45)	0.52 [0.54]
			$CmSC_3H_4^+$ (30)	
			$CmSC_5H_6^+$ (25)	

[a] Where more than one product was observed, the relative yields are given in parentheses as percentages; the pseudo-first-order rates are expressed as reaction efficiencies, k/k_{COL}, and in brackets as absolute rates, $k/10^{-9}$ cm^3 $molecule^{-1}$ s^{-1}.

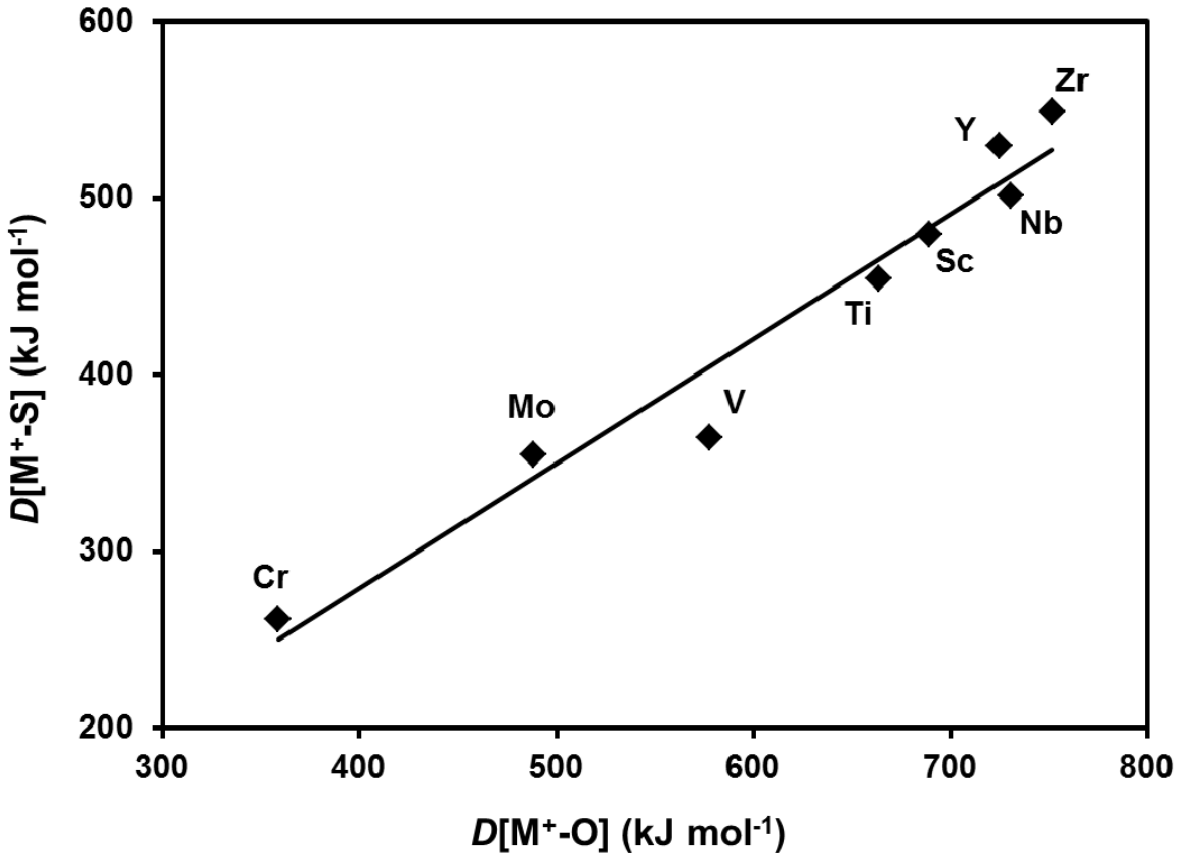

Fig. S1 Plot of $D_0[M^+\text{-}S]^{1\text{-}5}$ versus $D_0[M^+\text{-}O]^6$ for early first and second row transition metal cations (the linear fit has a $R^2 = 0.956$).

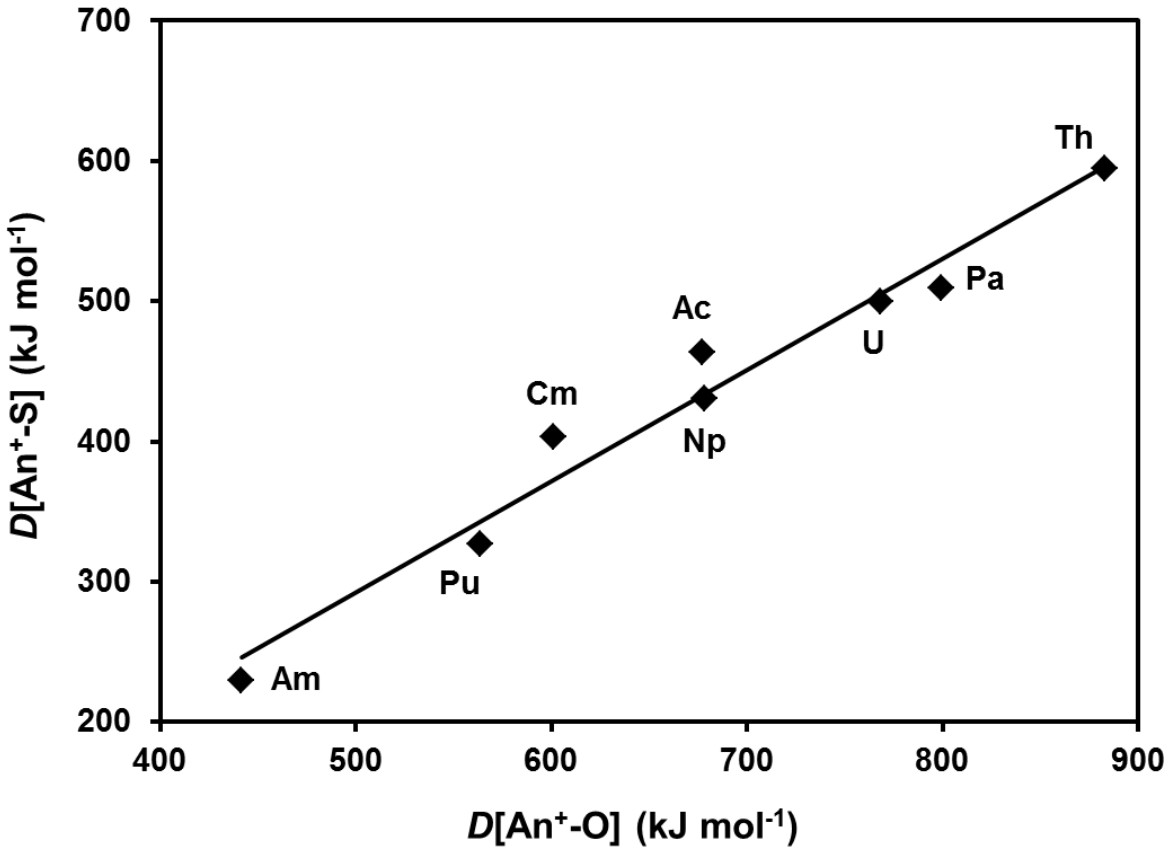

Fig. S2 Plot of the average computed values of $D[An^{+}\text{-}S]$ versus $D[An^{+}\text{-}O]$ (the linear fit has a R^2 = 0.968).

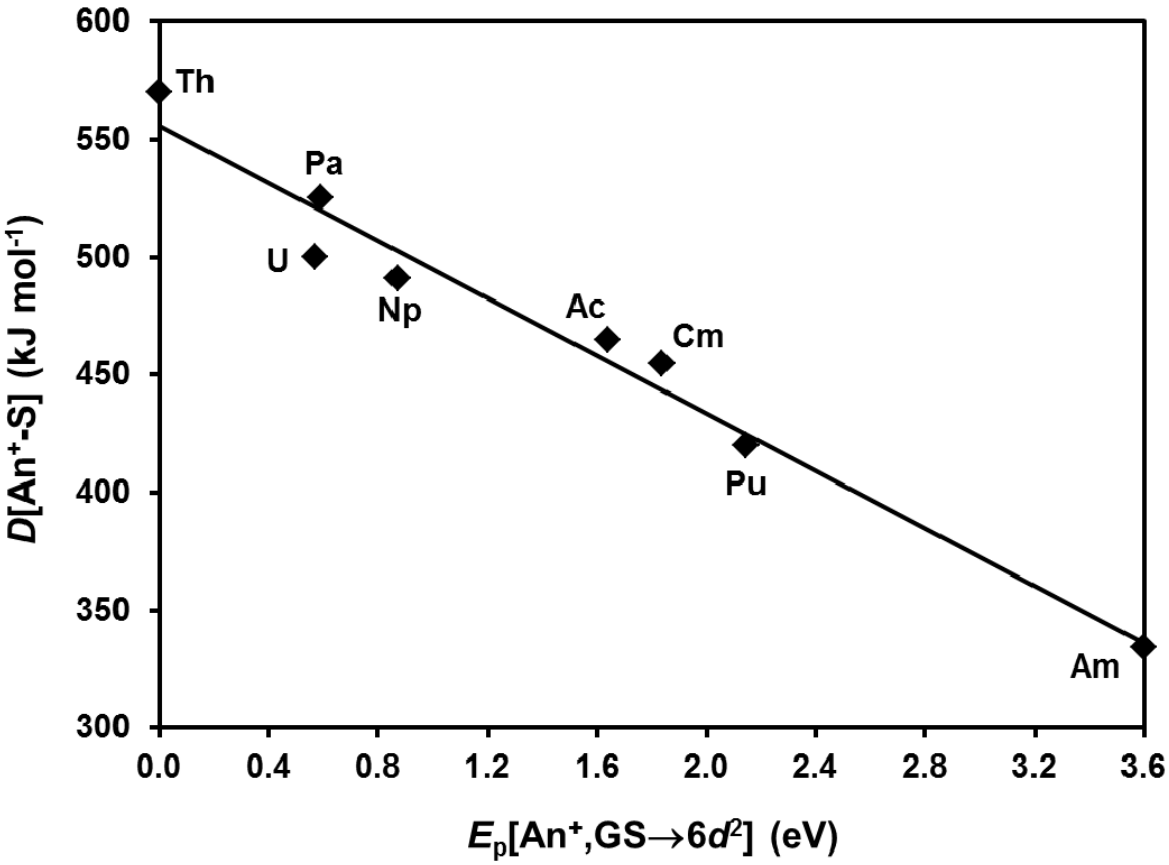

Fig. S3 Plot of $D[An^+\text{-}S]$ estimated in this work versus $E_p[GS \rightarrow 6d^2]$ of the An^+ ions[7] (the linear fit has a $R^2 = 0.970$).

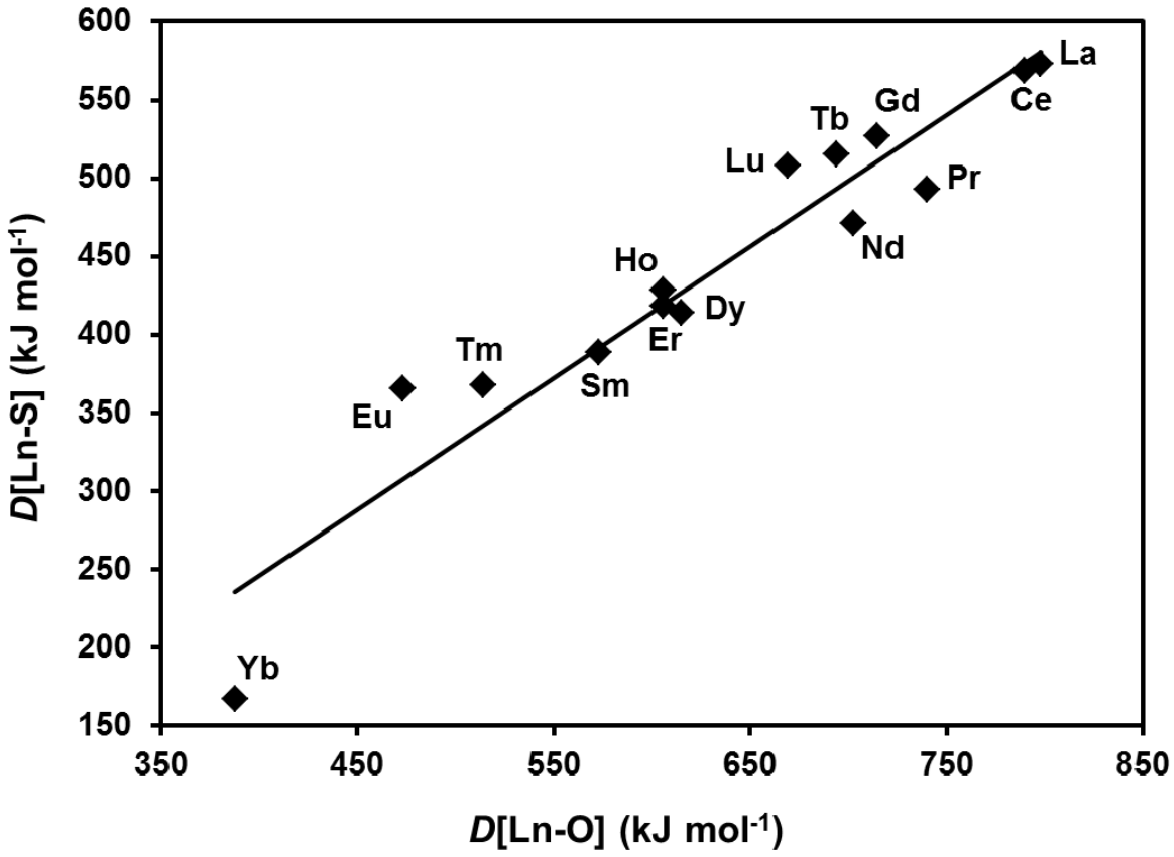

Fig. S4 Plot of D[Ln-S][8] versus D[Ln-O][8] for the lanthanide metals (the linear fit has a $R^2 = 0.905$). The D[Yb-S] point is clearly an outlier; see ref. 9 for additional information.

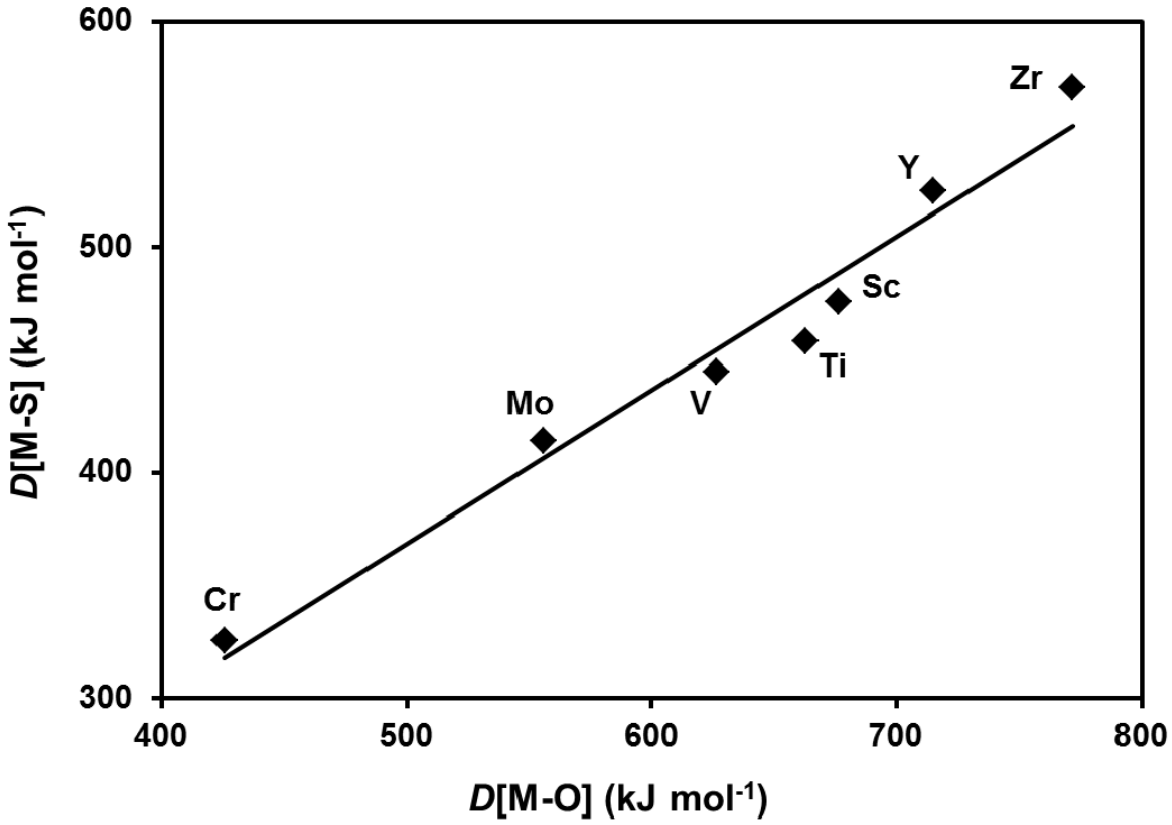

Fig. S5 Plot of D_0[M-S]^6 versus D_0[M-O]^6 for early first and second row transition metals (the linear fit has a $R^2 = 0.967$).

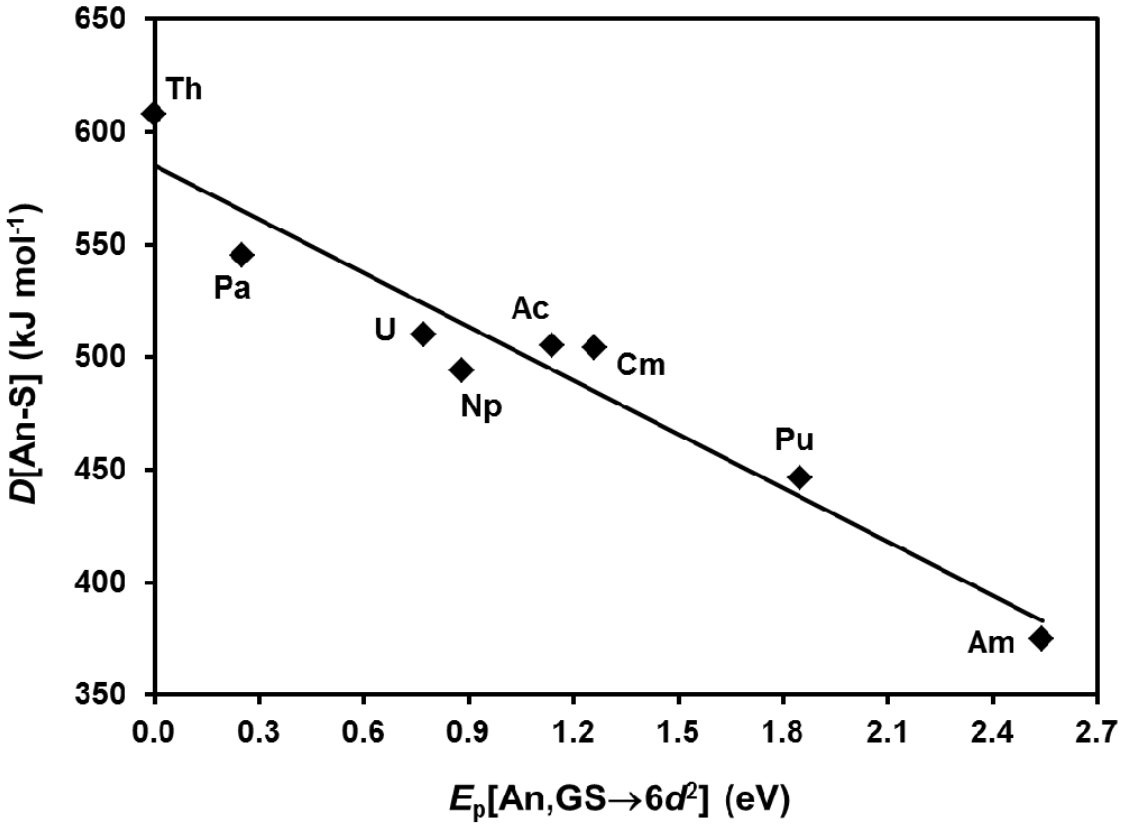

Fig. S6 Plot of D[An-S] estimated in this work versus E_p[GS → $6d^2$] of the An neutral atoms[7] (the linear fit has a $R^2 = 0.933$).

References

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