Supplementary material: Polynomial expansion coefficients in internal coordinates of the 6D-PES of $N_2HAr^+(X^1\Sigma^+)$, obtained at the *spdf(g)* aug-cc-pV5Z/CCSD(T) level and including the BSSE correction. The definition of the c_{ijklmn} terms is given in equation (1).

c_{ijklmn}		c_{ijklmn}		c_{ijklmn}		c_{ijklmn}		c_{ijklmn}		c_{ijklmn}	
000000	0.0[a)]	100000	-0.00502497	200000	3.24390207	300000	-2.32055147	400000	-2.89730896	010000	-0.00012543
110000	-0.05023397	210000	-0.03539725	310000	-0.08483021	020000	0.62227651	120000	-0.03921439	220000	-0.37701795
030000	-0.27643395	130000	-0.21908102	040000	-0.16322893	001000	0.00344940	101000	-0.00494303	201000	-0.25974512
301000	0.04972400	011000	0.27197594	111000	-0.03497321	211000	1.13180466	021000	0.44611419	121000	0.32942036
031000	0.19111225	002000	0.13810980	102000	-0.17156890	202000	-1.95793336	012000	-0.41673523	112000	-0.49605559
022000	1.50533523	003000	-0.22305652	103000	-0.19662179	013000	0.63540098	004000	0.06102776	000200	0.02433309
100200	-0.09498732	200200	-0.07310182	010200	-0.02247271	110200	0.05187652	020200	0.05147591	001200	0.00796196
101200	-0.09533960	011200	0.03929762	002200	0.03530428	000400	0.00149076	000020	0.00789444	100020	-0.00450830
200020	-0.03623731	010020	-0.00645737	110020	-0.04606385	020020	0.04423372	001020	-0.05122637	101020	-0.02890326
011020	0.11479287	002020	0.12157904	000220	0.00461515	000040	0.00380934	000111	-0.00567112	100111	0.00909637
200111	0.02015904	010111	0.01392668	110111	0.05277127	020111	-0.09102641	001111	0.01187686	101111	0.02184742
011111	-0.09147034	002111	-0.09779185	000311	0.01171510	000131	0.01171477	000222	0.00134021		

a) Total CCSD(T) energy at the equilibrium geometry of $N_2HAr^+(X^1\Sigma^+)$: -636.70018444 E_h. The equilibrium geometry is R_1=1.093888 Å, R_2=1.071154 Å and R_3=1.920110 Å.