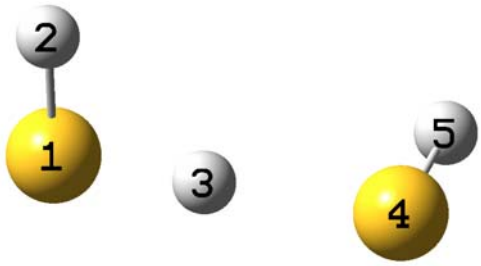
Supporting information

The energies and corresponding geometry parameters of the fully optimized and the constraint anionic structure were calculated with Molpro at the RCCSD(T)/aug-cc-pVTZ level and are given in Table 1:



	minimum	constraint
1-3 [Å]	1.432	1.433
1-4 [Å]	2.050	2.050
1-2 [Å]	1.342	1.345
4-5 [Å]	1.347	1.345
1-4-3 [°]	0.2	0.0
2-1-3 [°]	92.5	92.3
3-4-5 [°]	90.7	92.3
2-1-4-5 [°]*	89.4	89.4
Energy [eV]	-21696.62517248	-21696.62517248

The ab-initio energies have been fitted with a polynomial of 8th order up to 6 eV with respect to the reference energy:

$$V(x) = a_0 + a_1 * x^2 + a_2 * x^4 + a_3 * x^6 + a_4 * x^8$$

The fitted parameters are listed in Table 2:

	anion	neutral molecule
a	0.0	3.37304
a_1	-2.27516	-6.50658
a_2	11.455	22.602
a_3	3.53403	-11.0417
a_4	4.29274	11.6663

A standard deviation of $5.3*10^{-4}$ eV (17 points) for the anion potential and $6.3*10^{-3}$ eV (38 points) for the molecular potential were obtained.