Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Exploring Chemical Space with Alchemical Derivatives: Alchemical Transformations of H through Ar and its Ions as a Proof of Concept.

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Alchemical derivatives up to third order ($\mu^{al}, \eta^{al}, \gamma^{al}$) for the di-cations, mono-cations, neutral and mono-anions of the atoms H-Ar.
All values were obtained at the CAMB3LYP aug-cc-pCVQZ level of theory.

	μ^{al} [eV]				η^{al} [eV]				γ^{al} [meV]			
	$Q = Z - N$				$Q = Z - N$				$Q = Z - N$			
	+2	+1	0	-1	+2	+1	0	-1	+2	+1	0	-1
H			-26.96	-37.84			-27.03	-50.98			-0.987	-21.657
He		-54.20	-91.52	-98.72		-27.27	-54.27	-54.64		0.149	-0.148	-3.312
Li	-81.47	-145.99	-153.56	-160.35	-27.25	-54.46	-61.68	-69.75	0.036	-0.111	0.742	1.899
Be	-200.47	-215.02	-229.09	-233.20	-54.44	-61.30	-68.18	-79.08	-0.046	0.068	0.464	-31.609
B	-276.31	-297.23	-309.98	-317.18	-61.26	-68.02	-75.16	-83.92	0.008	0.166	0.444	1.129
C	-365.30	-385.06	-399.97	-409.46	-67.99	-74.95	-82.10	-90.25	0.120	0.168	0.440	0.744
N	-460.01	-481.97	-499.03	-508.95	-74.87	-81.85	-89.03	-97.41	0.084	0.189	0.462	-0.278
O	-563.79	-587.93	-605.72	-617.78	-81.74	-88.74	-96.07	-104.42	0.080	0.223	0.701	0.498
F	-676.63	-701.59	-721.50	-735.68	-88.59	-95.67	-103.03	-111.42	0.096	0.286	0.747	1.027
Ne	-797.19	-824.31	-846.35	-855.14	-95.47	-102.59	-109.98	-111.29	0.157	0.303	0.791	1.493
Na	-926.81	-956.14	-964.30	-968.92	-101.61	-108.71	-112.81	-119.31	0.739	0.973	2.889	8.576
Mg	-1065.43	-1077.31	-1086.68	-1089.84	-107.35	-110.77	-114.72	-121.38	1.734	2.343	3.032	-18.773
Al	-1189.94	-1202.91	-1211.44	-1216.80	-112.20	-115.63	-119.55	-125.39	0.547	0.776	1.541	4.747
Si	-1318.53	-1330.71	-1340.53	-1347.49	-115.33	-118.79	-122.58	-127.43	0.460	0.701	1.266	3.212
P	-1449.44	-1462.84	-1473.92	-1481.42	-118.46	-121.89	-125.58	-130.32	0.414	0.634	1.070	2.287
S	-1584.65	-1599.26	-1610.90	-1619.72	-121.55	-124.96	-128.68	-133.22	0.379	0.580	1.014	2.327
Cl	-1724.14	-1739.33	-1752.18	-1762.29	-124.63	-128.05	-131.74	-136.14	0.356	0.567	0.941	2.164
Ar	-1867.29	-1883.68	-1897.75	-1904.03	-127.71	-131.14	-134.80	-135.68	0.359	0.550	0.888	1.100