

The Halogen-Bond Nature in Noble Gas-Dihalogen Complexes from Scattering Experiments and Ab-Initio Calculations

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Supporting Materials

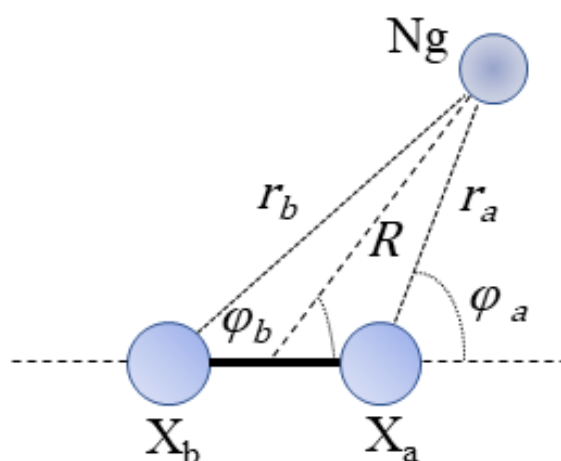


Figure S1. Coordinate systems for the Ng-X₂ systems case study.

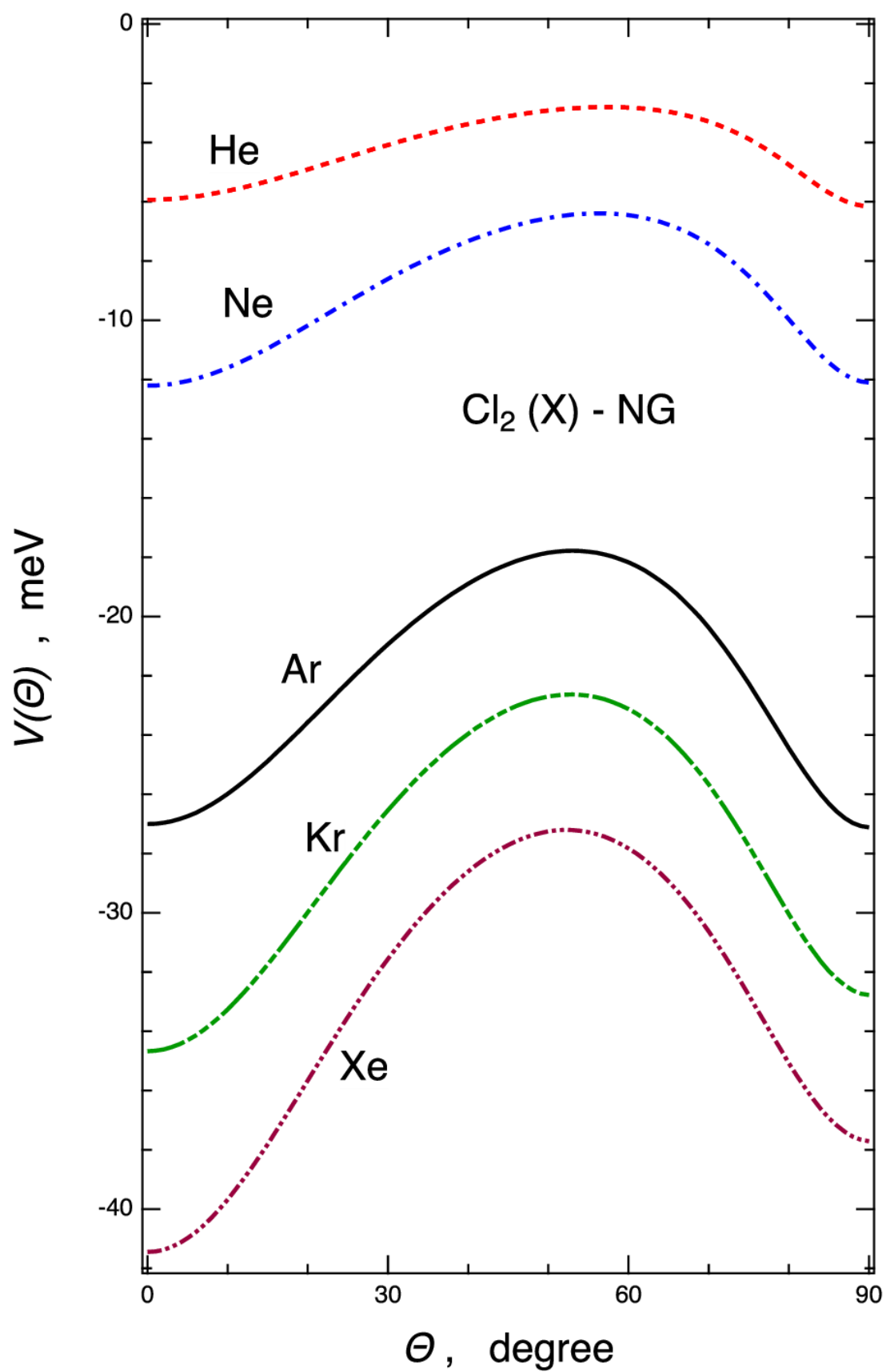


Figure S2. Angular MEP for the Ng-Cl₂ complexes in the ground X state of Cl₂, reporting the interaction energy, as derived from the potential parametrization, vs the angular variable Θ .

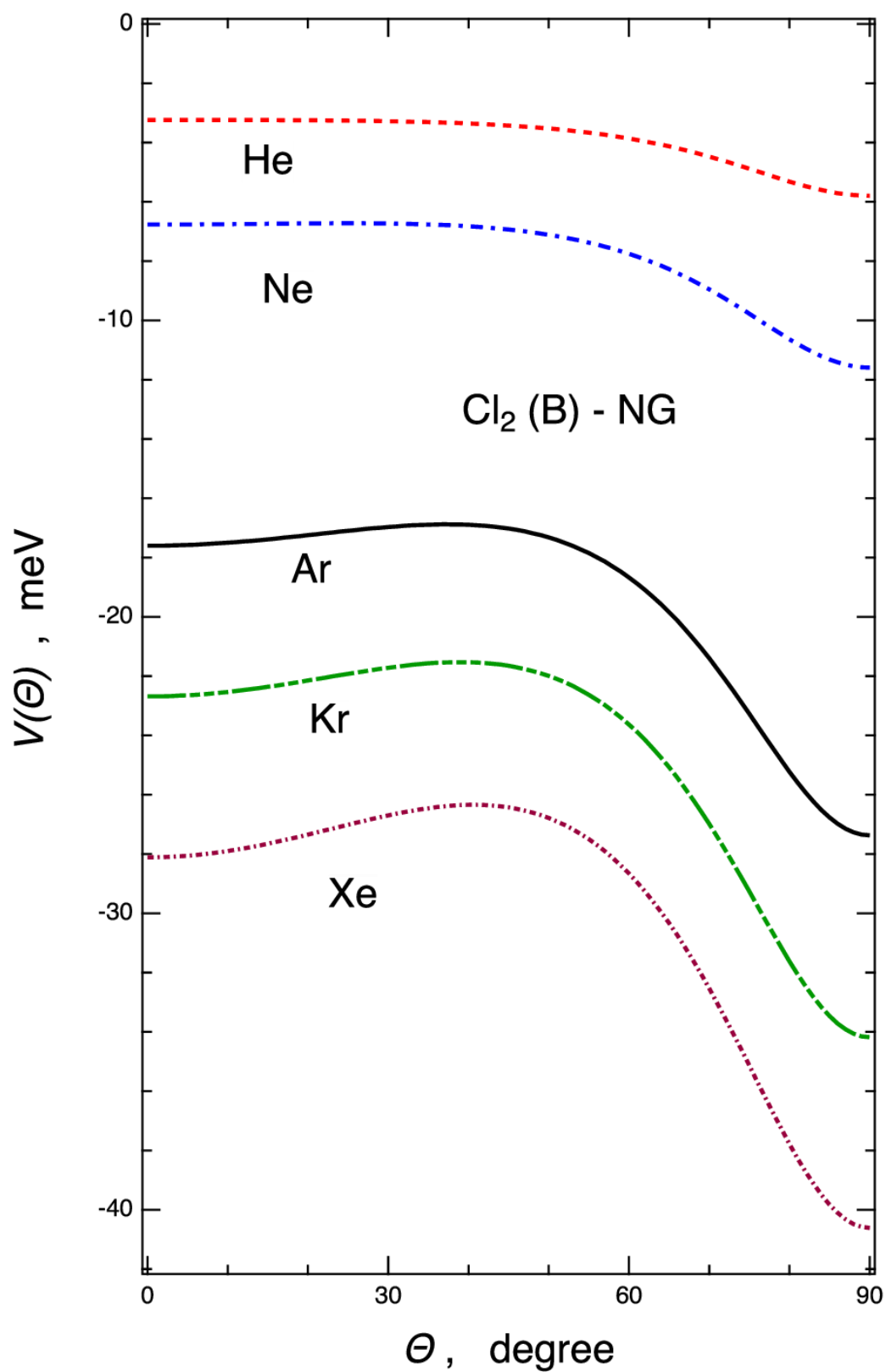


Figure S3. Angular MEP for the Ng-Cl₂ complexes in the excited *B* state of Cl₂, reporting the interaction energy, as derived from the potential parametrization, vs the angular variable Θ .

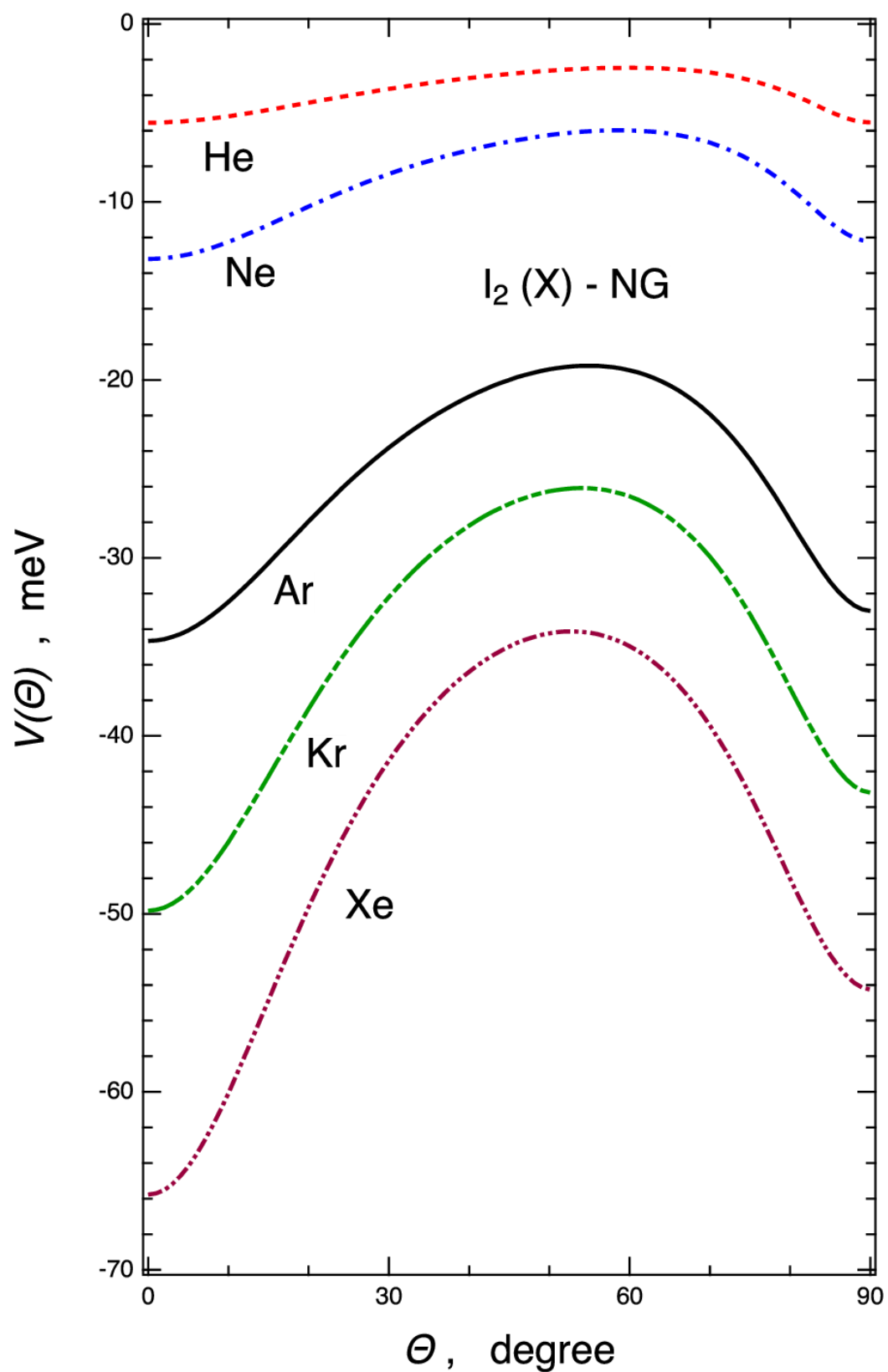


Figure S4. Angular MEP for the Ng-I₂ complexes in the ground X state of I₂, reporting the interaction energy, as derived from the potential parametrization, vs the angular variable Θ .

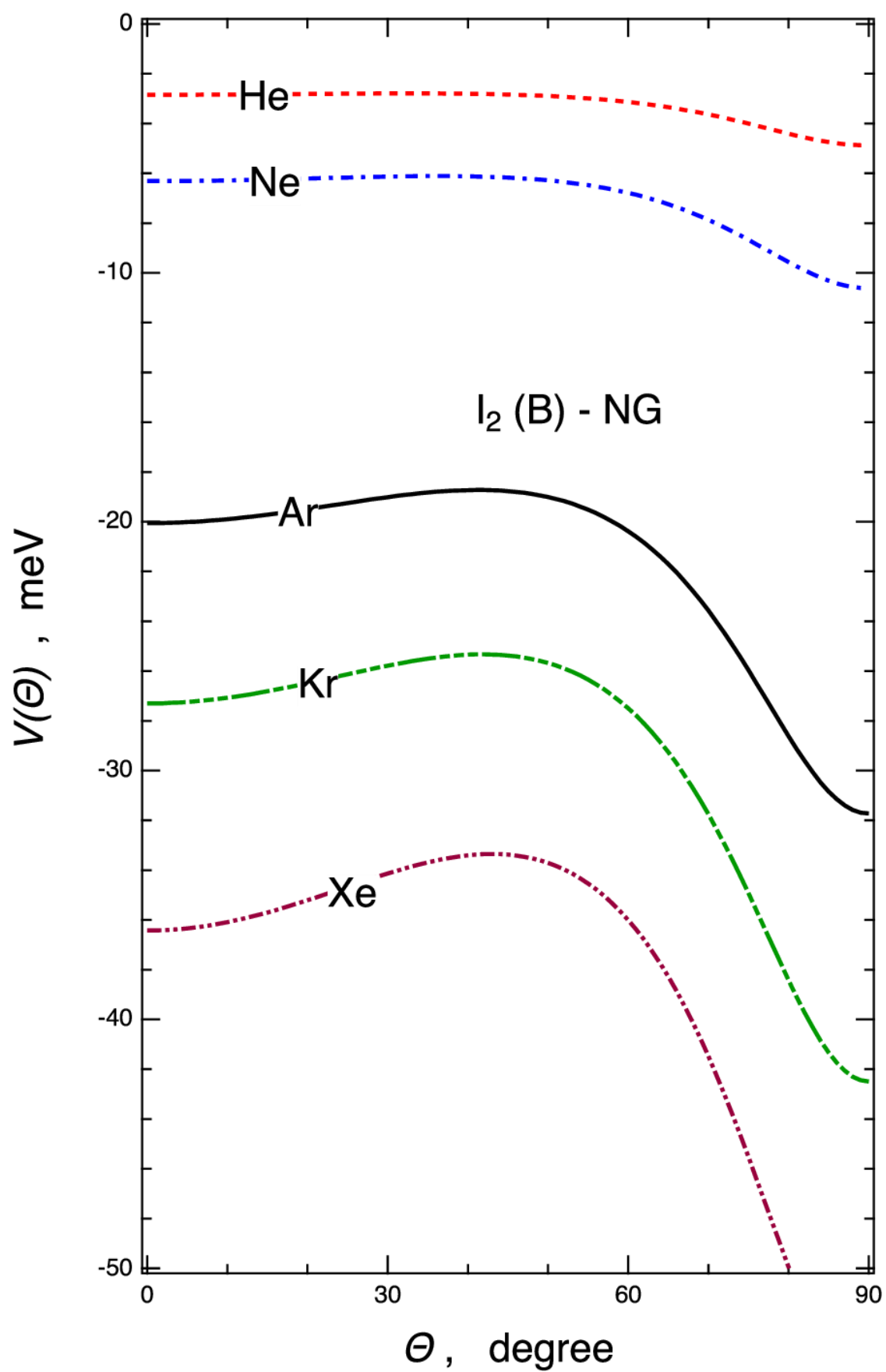


Figure S5. Angular MEP for the Ng- I_2 complexes in the excited B state of I_2 , reporting the interaction energy, as derived from the potential parametrization, vs the angular variable Θ .

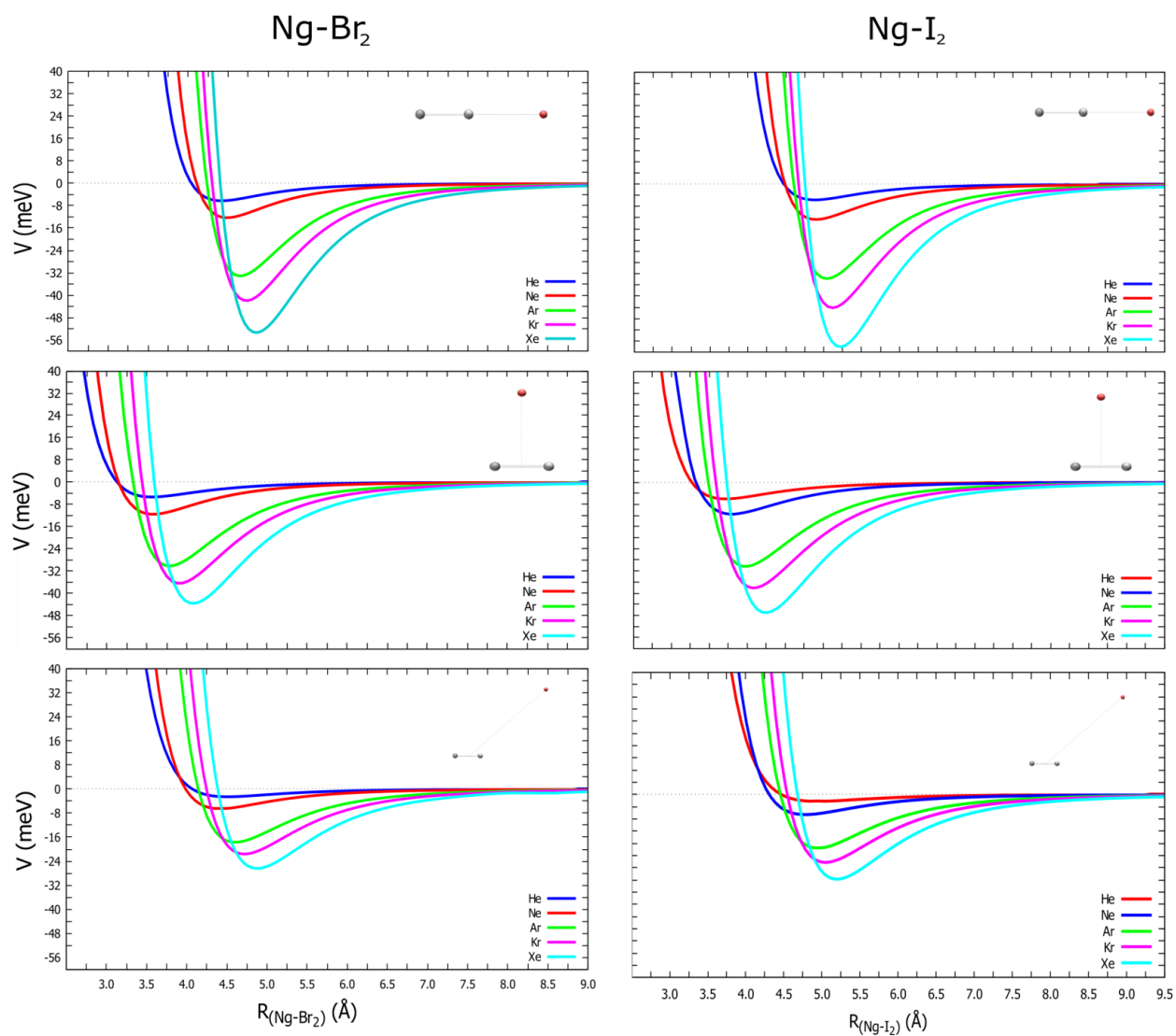


Figure S6. CCSD(T) potential energy curves (interaction potential V vs. Ng-Br₂ distance R) for the ground state Ng-Br₂ (AV5Z) and Ng-I₂ (AVQZ) complexes.

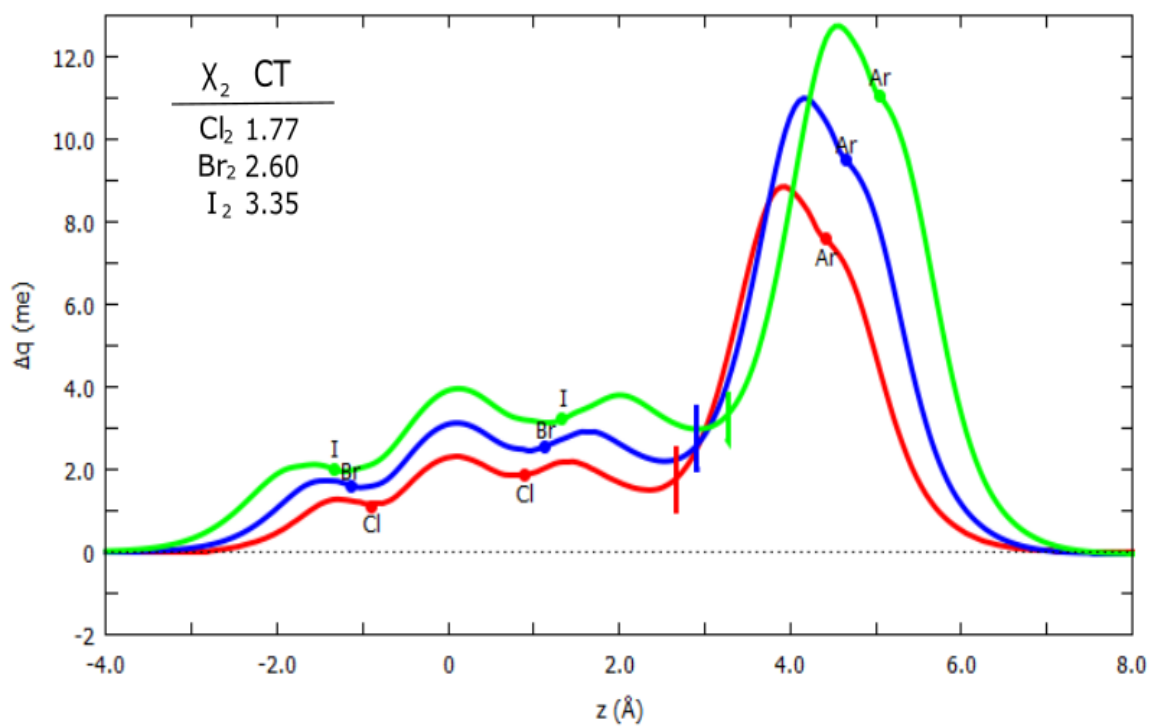


Figure S7. Charge displacement functions (CCSD/AVQZ) of Ar-X₂ (X $^1\Sigma_g^+$) complexes in the linear configuration. Dots on graphs represent the position in the z -axis of the different atoms nuclei. Vertical lines are the isodensity boundary.

Table S1. Equilibrium distances R_m (Å) and binding energy values E_m (meV) for Ng-Br₂ complexes in both ground ($X^1\Sigma_g^+$) [CCSD(T)/AVXZ, X = T, Q, 5] and excited ($B^3\Pi_u$) [UCCSD(T)/AVTZ] states in the three relative configurations (linear, T-shaped, saddle). In parenthesis the energy values with BSSE corrections.

	Linear		T-Shaped		Saddle (50°)	
Basis	R_m	E_m	R_m	E_m	R_m	E_m
He-Br₂ ($X^1\Sigma_g^+$)						
AVTZ	4.46	6.73 (4.61)				
AVQZ	4.43	6.21 (5.36)	3.57	5.33 (4.70)	4.52	2.58 (2.41)
AV5Z	4.42	6.27 (5.67)	3.56	5.35 (5.02)	4.51	2.58 (2.41)
Ne-Br₂ ($X^1\Sigma_g^+$)						
AVQZ	4.48	13.21 (10.03)	3.57	12.06 (9.59)	4.41	7.02 (5.35)
AV5Z	4.48	12.31 (10.83)	3.57	11.57 (10.49)	4.42	6.56 (5.86)
Ar-Br₂ ($X^1\Sigma_g^+$)						
AVTZ	4.71	31.41	3.83	28.75	4.64	17.54
AVQZ	4.66	32.35 (28.62)	3.79	29.16 (26.40)	4.62	17.29 (15.25)
AV5Z	4.65	33.10 (30.38)	3.78	30.22 (28.07)	4.60	17.71 (16.31)
Kr-Br₂ ($X^1\Sigma_g^+$)						
AVQZ	4.75	41.00 (37.18)	3.91	35.59 (32.73)	4.73	21.31 (19.36)
AV5Z	4.72	41.66 (39.06)	3.90	36.45 (34.76)	4.72	19.15 (18.40)
Xe-Br₂ ($X^1\Sigma_g^+$)						
AVQZ	4.86	52.20	4.09	42.41	4.89	25.86
AV5Z	4.85	53.36	4.07	43.67	4.88	26.41
Ar-Br₂ ($B^3\Pi_u$)						
AVTZ	5.29	18.80	3.84 ^(a)	25.79 ^(a)	4.60 ^(c)	20.39 ^(c)
			3.82 ^(b)	27.00 ^(b)	4.77 ^(d)	16.78 ^(d)

^(a) B₂ symmetry. ^(b) A₁ symmetry.

Table S2. V_{CT} components and CT constant k evaluated at the optimized equilibrium distances (R_{Ng-X_2} , Å).

Ng	R_{Ng-cl_2}	V_{CT}	k	R_{Ng-Br_2}	V_{CT}	k	R_{Ng-I_2}	V_{CT}	k
He	4.11	1.73	5.00	4.43	2.34	4.84	4.88	2.21	4.02
Ne	4.20	3.66	5.16	4.48	5.34	5.18	4.90	5.77	4.58
Ar	4.40	7.23	5.09	4.66	11.41	4.39	5.04	13.99	4.18
Kr	4.52	12.27	5.00	4.75	17.82	4.73	5.12	22.02	4.45
Xe	4.66	15.14	4.55	4.86	24.91	4.46	5.22	31.71	4.16