Supporting Information

Exponential Relationships Capturing Atomistic Short-Range Repulsion from the Interacting Quantum Atoms (IQA) Method

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$$E^{AB}_{Deformation} = Ae^{-Br} \qquad (10)$$

$$E^{AB}_{Deformation} = Ae^{-Br+Cr^2} \qquad (11)$$

	Ae^{-Br+Cr^2}			Ae^{-Br}	
System	**A**	**B**	**C**	**A**	**B**
He_He	1184.20	2.65	-3.55	10919.76	8.29
Ne_Ne	97718.87	11.36	1.62	35541.92	8.79
Ar_Ar	494825.28	14.30	4.09	34657.49	7.67
He_Ne	11448.23	7.44	-0.53	15993.25	8.28
He_Ar	39105.17	10.19	1.80	12089.82	7.27
Ne_Ar	378544.91	14.28	3.86	31793.86	8.06
H2_H2	689.06	2.90	-2.13	2896.30	6.42
N2_N2	60649.10	8.32	0.65	39671.82	7.26
NH3_NH3	15509.53	4.59	-1.46	40837.98	6.99
O2_O2	10555.48	6.24	0.79	5893.22	4.87
OH2_OH2	2393.06	0.01	-5.18	62573.39	8.27
F2_F2	13768.93	5.26	-3.01	84484.97	9.95
FH_FH	217451.26	12.78	3.41	22845.50	7.20
S2_S2	106456.32	10.49	3.31	9049.39	4.70
SH2_SH2	116453.81	9.45	1.63	39298.20	6.77
Cl2_Cl2	3926.68	-0.20	-6.55	202283.94	10.00
ClH_ClH	263666.41	11.09	1.68	91525.89	8.41
OH2_H2	17637.28	8.46	2.08	3809.89	4.85
OH2_N2	87822.24	9.88	2.09	21173.94	6.41
OH2_NH3	8228.67	3.20	-2.63	45452.01	7.47

OH2_O2	97185.81	11.06	2.96	12559.05	6.10
H2_N2	5564.15	4.91	-0.95	10543.13	6.48
H2_F2	897.34	1.83	-3.86	10403.28	8.01
H2_FH	23051.13	9.70	2.62	3477.00	5.21
NH3_FH	67206.15	9.07	1.29	28594.64	6.96
F2_FH	332262.30	14.58	4.72	13729.52	6.76
OH2_FH	69312.46	9.27	1.04	35329.15	7.59
NH3_H2	10771.08	7.01	1.39	3833.15	4.58
OH2_ClH	191286.96	11.30	2.73	30671.21	6.80
N2_S2	36252.01	6.82	-0.47	49232.78	7.58
N2_SH2	53433.33	7.85	0.57	36715.19	6.92
OH2_Cl2	194985.41	11.91	3.42	18375.41	6.17
OH2_F2	117200.33	12.19	3.75	8371.29	5.84
OH2_S2	146501.36	11.11	3.10	16696.19	5.87
OH2_SH2	140105.36	10.56	2.67	21966.24	6.07