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Quantitative Evaluation of Anharmonic Bond Potentials for Molecular Simulations - Supporting Information

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Table S1 Name and properties (charge q, multiplicity m) of the diatomics studied. Covalency is indicated by cov. Equilibrium distance r_{eq} [1], range of the quantum chemical scan (r_0, r_1 in Å) and number of points N in the scan.

Compound	Formula	q	m	cov	r_0	r_{eq}	r_1	N
dicarbon	C_2	0	1	True	1.04	1.24253	1.49	89
carbon monofluoride	CF	0	2	True	1.07	1.2718	1.525	92
carbon monohydride	CH	0	2	True	0.94	1.1199	1.34	72
dilithium	Li_2	0	1	True	2.25	2.6729	3.205	190
lithium hydride	LiH	0	1	True	1.34	1.59491	1.91	114
cyano radical	CN	0	2	True	0.98	1.17182	1.405	81
nitrogen ion	N_2^+	1	2	True	0.92	1.11642	1.315	71
hydrogen	H_2	0	1	True	0.62	0.74144	0.885	55
hydrogen fluoride	HF	0	1	True	0.77	0.916808	1.1	60
hydrogen chloride	HCl	0	1	True	1.07	1.27455	1.525	92
hydrogen bromide	HBr	0	1	True	1.19	1.41444	1.695	103
hydrogen iodide	HI	0	1	True	1.35	1.60916	1.93	116
fluorine	F_2	0	1	True	1.19	1.41193	1.69	102
chlorine	Cl_2	0	1	True	1.67	1.9879	2.375	122
bromine	Br_2	0	1	True	1.92	2.28105	2.735	147
chlorine fluoride	ClF	0	1	True	1.37	1.62831	1.95	116
bromine fluoride	BrF	0	1	True	1.48	1.75894	2.105	119
iodine fluoride	IF	0	1	True	1.6	1.9098	2.29	123
bromine chloride	BrCl	0	1	True	1.79	2.13606	2.56	131
iodine chloride	ICl	0	1	True	1.95	2.32088	2.785	153
iodine bromide	IBr	0	1	True	2.07	2.46899	2.96	172
iodine	I_2	0	1	True	2.24	2.6663	3.195	190
oxygen	O_2	0	3	True	1.01	1.20752	1.445	86
nitrogen	N_2	0	1	True	0.92	1.09769	1.315	71
carbon monoxide	CO	0	1	True	0.95	1.12832	1.35	72
carbon monosulfide	CS	0	1	True	1.29	1.53494	1.84	111
sulfur monoxide	SO	0	3	True	1.24	1.48109	1.775	108
phosphor nitride	PN	0	1	True	1.25	1.49087	1.785	108
hydroxide	OH^-	-1	1	True	0.81	0.97	1.155	61
hydroxide	OH	0	2	True	0.81	0.96966	1.155	61
nitric oxide	NO	0	2	True	0.97	1.15077	1.38	76
lithium fluoride	LiF	0	1	False	1.31	1.56386	1.875	114
lithium chloride	LiCl	0	1	False	1.7	2.02067	2.42	123
lithium bromide	LiBr	0	1	False	1.82	2.17043	2.6	134
lithium iodide	LiI	0	1	False	2.01	2.39192	2.87	162
sodium fluoride	NaF	0	1	False	1.62	1.92595	2.31	122
sodium chloride	NaCl	0	1	False	1.98	2.36079	3.03	198
sodium bromide	NaBr	0	1	False	2.1	2.50204	3	176
sodium iodide	NaI	0	1	False	2.28	2.71145	3.25	194
potassium fluoride	KF	0	1	False	1.82	2.17146	2.605	137
potassium chloride	KCl	0	1	False	2.24	2.66665	3.195	190
potassium bromide	KBr	0	1	False	2.37	2.821	3.38	202
potassium iodide	KI	0	1	False	2.56	3.04784	3.655	219
rubidium fluoride	RbF	0	1	False	1.91	2.27033	2.72	149
rubidium chloride	RbCl	0	1	False	2.34	2.78674	3.34	200
rubidium bromide	RbBr	0	1	False	2.47	2.945	3.53	212
rubidium iodide	RbI	0	1	False	2.67	3.17688	3.81	227
cesium fluoride	CsF	0	1	False	1.97	2.34535	2.81	156
cesium chloride	CsCl	0	1	False	2.44	2.90627	3.485	210
cesium bromide	CsBr	0	1	False	2.58	3.07225	3.685	221

Compound	Formula	q	m	cov	r_0	r_{eq}	r_1	N
cesium iodide	CsI	0	1	False	2.78	3.31519	3.975	237
beryllium oxide	BeO	0	1	False	1.12	1.3309	1.595	88
beryllium sulfide	BeS	0	1	False	1.46	1.74153	2.085	120
magnesium oxide	MgO	0	1	False	1.47	1.749	2.095	126
magnesium sulfide	MgS	0	1	False	1.8	2.1425	2.57	131
calcium oxide	CaO	0	1	False	1.53	1.8221	2.145	108
calcium sulfide	CaS	0	1	False	1.95	2.3178	2.78	154
boron monofluoride	BF	0	1	True	1.06	1.26259	1.52	92
boron monochloride	BCl	0	1	True	1.44	1.7159	2.06	120
bromine monoxide	BrO	0	2	True	1.44	1.717	2.06	120
chlorine monoxide	ClO	0	2	True	1.34	1.56963	1.915	115
iodine monoxide	IO	0	2	True	1.57	1.8676	2.24	122
lithium monoxide	LiO	0	2	True	1.42	1.695	2.025	119
nitric oxide ion	NO^+	1	1	True	0.9	1.06322	1.27	66
nitric sulfide	NS	0	2	True	1.26	1.49402	1.795	108
sodium hydride	NaH	0	1	True	1.58	1.889	2.25	121
phosphorus monofluoride	PF	0	3	True	1.34	1.5897	1.91	114
phosphorus monoxide	PO	0	2	True	1.24	1.4759	1.77	107
sulfur monofluoride	SF	0	2	True	1.34	1.59624	1.915	115
sulfur hydride	SH	0	2	True	1.13	1.3409	1.605	97
disulfur	S_2	0	3	True	1.63	1.8892	2.325	122

Table S2 Statistics per function for quantum chemistry results. M_f is the number of parameters used for fitting, M_{sim} the number of parameters if the minimum is not fixed at zero and when redundancies are removed (see text). N is the number of compounds, Z is the average Z-score ($cm^{-2}/Å$), and RMSD (J/mol) is the root mean signed error from quantum results. No energy cut-off was applied. Table is sorted after Z-score for covalent compounds computed at the CCSD(T) level of theory.

			CCSD(T)				MP2			
			Non-covalent (26)		Covalent (45)		Non-covalent (26)		Covalent (45)	
Function	M_f	M_{sim}	Z	RMSD	Z	RMSD	Z	RMSD	Z	RMSD
Sun[2]	8	8	1.1	10	0.0	1.6	4.0	19	362	181
Hulburt-Hirschfelder[3]	5	5	6.1	24	0.5	6.7	21	44	475	201
Rafi[4]	5	4	29	55	4.5	20	123	106	2480	448
Tietz II[5]	5	4	23	51	6.2	23	130	110	4640	605
Wei Hua[6]	4	4	25	54	6.7	24	140	114	6240	701
Levine[7]	4	4	36	64	12	33	458	205	6645	724
Frost-Musulin[8]	4	3	142	125	140	102	599	239	6488	713
Pöschl-Teller[9]	4	3	146	128	171	114	603	240	6553	717
Cahill[10]	6	6	19	43	199	125	25	43	4005	564
Linnett[11]	4	3	165	134	238	129	493	220	6174	695
Murrell-Sorbie[12]	5	5	148	115	291	146	376	180	7990	786
Morse[13]	3	3	199	150	323	154	771	272	9443	859
Deng-Fan[14]	3	3	191	141	360	149	905	292	9070	836
Valence-State[15]	4	4	245	157	553	205	719	261	7290	748
Rosen-Morse[16]	4	3	205	152	563	201	621	246	7231	754
Rydberg[17]	3	3	247	169	634	217	808	282	9644	870
Varshni[18]	3	3	314	194	1020	282	935	305	9388	861
Pseudo-Gaussian[19]	3	3	418	224	1613	353	977	317	10071	893
Tang2003a[20]	6	6	1516	469	5937	562	1547	384	75357	2255
Buckingham[21]	3	3	1458	382	8931	752	3999	615	19362	1172
Tietz I[5]	5	4	283	174	11019	1019	1069	320	17928	1107
Wang-Buckingham[22]	3	3	2454	505	15804	1031	3731	611	24275	1351
Noorizadeh[23]	5	4	1413	343	128209	2951	2430	458	136069	3062
Kratzer[24]	2	2	48819	2366	217453	4168	41893	2224	243383	4267
Lippincott[25]	3	3	186617	4551	905299	8215	171882	4396	937451	8230
Xie2005a[26]	4	3	200963	4634	1235501	9549	193001	4561	1211337	9372
Harmonic	3	2	421985	6801	2102933	12378	409422	6710	2137866	12347
Lennard-Jones[27]	2	2	595164	7933	3556003	15521	768761	8865	3435437	15369

Table S3 Statistics per function for quantum chemistry results. M_f is the number of parameters used for fitting, M_{sim} the number of parameters if the minimum is not fixed at zero and when redundancies are removed (see text). N is the number of compounds, Z is the average Z-score ($cm^{-2}/Å$), and RMSD (J/mol) is the root mean signed error from quantum chemical results. An energy cut-off of 5000 cm^{-1} was applied. Table is sorted after Z-score for covalent compounds computed at the CCSD(T) level of theory.

			CCSD(T)				MP2			
			Non-covalent (26)		Covalent (45)		Non-covalent (26)		Covalent (45)	
Function	M_f	M_{sim}	Z	RMSD	Z	RMSD	Z	RMSD	Z	RMSD
Sun[2]	8	8	0.2	4.3	0.0	0.3	0.2	3.8	31	52
Hulburt-Hirschfelder[3]	5	5	2.9	15	0.0	1.2	7.9	25	106	94
Tietz II[5]	5	4	14	37	0.6	6.4	29	50	256	133
Wei Hua[6]	4	4	24	46	0.6	6.7	31	51	304	143
Cahill[10]	6	6	4.2	21	3.1	15	26	43	389	174
Levine[7]	4	4	22	47	4.6	21	130	90	586	211
Frost-Musulin[8]	4	3	50	74	16	32	198	129	549	197
Pöschl-Teller[9]	4	3	56	79	19	34	207	132	555	198
Morse[13]	3	3	88	99	35	45	288	158	686	214
Linnett[11]	4	3	55	78	37	45	218	136	497	183
Murrell-Sorbie[12]	5	5	24	49	38	46	44	59	305	136
Rosen-Morse[16]	4	3	89	99	48	52	234	144	571	198
Rydberg[17]	3	3	120	117	51	54	303	166	696	216
Valence-State[15]	4	4	42	63	52	61	244	139	589	202
Varshni[18]	3	3	162	135	80	67	342	177	751	226
Deng-Fan[14]	3	3	50	74	90	66	337	159	823	235
Tietz I[5]	5	4	76	88	93	80	375	174	526	174
Pseudo-Gaussian[19]	3	3	210	154	94	75	353	186	732	223
Wang-Buckingham[22]	3	3	982	322	1258	261	1153	342	1953	333
Buckingham[21]	3	3	410	199	1337	269	714	246	3029	436
Tang2003a[20]	6	6	127	108	2118	295	463	194	5482	486
Rafi[4]	5	4	14	36	3607	485	23	44	345	167
Noorizadeh[23]	5	4	813	251	15198	871	889	261	12490	791
Kratzer[24]	2	2	17225	1334	23327	1215	16488	1324	22094	1102
Lippincott[25]	3	3	55032	2390	69416	1990	53632	2386	68641	1924
Xie2005a[26]	4	3	58569	2411	98534	2374	55927	2382	95475	2261
Harmonic	3	2	127283	3592	193948	3336	122264	3554	186122	3176
Lennard-Jones[27]	2	2	178020	4179	360340	4364	195436	4296	380264	4534

Table S4 Vibrational harmonic frequency ω_e (1/cm), First anharmonic correction $\omega_e x_e$ (1/cm), Equilibrium rotational constant B_e (1/cm), First correction of the rotational constant α_e (1/cm), Centrifugal distortion constant D_e (1/cm), from experiment[1] and quantum chemistry (this work).

	Experiment					CCSD(T)					MP2				
Compound	ω_e	$\omega_e x_e$	B_e	α_e	D_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e
BeO	1487.3	11.83	1.65	1.90e-02	8.20e-06	1489.3	13.59	1.64	1.97e-02	7.98e-06	1428.7	14.00	1.62	2.09e-02	8.27e-06
BeS	997.9	6.14	0.79	6.64e-03	2.00e-06	1001.5	6.17	0.78	6.38e-03	1.92e-06	1011.0	4.82	0.78	5.86e-03	1.89e-06
BCl	839.1	5.11	0.68	6.46e-03	1.72e-06	857.3	7.11	0.68	7.03e-03	1.74e-06	877.1	7.19	0.69	7.04e-03	1.73e-06
BF	1402.1	11.84	1.51	1.98e-02	7.60e-06	1408.0	13.92	1.51	1.93e-02	6.91e-06	1419.3	13.95	1.51	1.93e-02	6.89e-06
Br_2	325.3	1.08	0.08	3.19e-04	2.09e-08	328.0	1.18	0.08	3.11e-04	1.99e-08	347.5	1.02	0.08	2.84e-04	1.89e-08
BrCl	444.3	1.84	0.15	7.70e-04	7.18e-08	442.0	2.08	0.15	7.66e-04	6.92e-08	466.9	1.79	0.15	7.02e-04	6.59e-08
BrF	670.8	4.05	0.36	2.61e-03	4.01e-07	683.7	4.55	0.36	2.67e-03	3.88e-07	701.9	4.04	0.36	2.50e-03	3.76e-07
BrO	778.7	6.80	0.43	3.64e-03	5.23e-07	738.3	5.83	0.43	3.80e-03	5.81e-07	685.2	3.13	0.44	2.99e-03	7.13e-07
CaO	732.1	4.81	0.44	3.38e-03	6.58e-07	593.0	8.11	0.41	5.42e-03	8.08e-07	675.3	7.69	0.43	3.97e-03	6.78e-07
CaS	462.2	1.78	0.18	8.37e-04	1.02e-07	433.9	1.99	0.17	8.71e-04	1.01e-07	443.3	2.00	0.17	8.66e-04	1.01e-07
CF	1308.1	11.10	1.42	1.84e-02	6.50e-06	1321.9	13.86	1.42	1.91e-02	6.49e-06	1342.5	13.79	1.43	1.90e-02	6.43e-06
CH	2858.5	63.02	14.46	5.34e-01	1.45e-03	2920.8	83.63	14.73	6.05e-01	1.50e-03	3017.2	76.70	14.92	5.57e-01	1.46e-03
CS	1285.1	6.46	0.82	5.92e-03	1.43e-06	1281.6	7.20	0.81	6.01e-03	1.30e-06	1308.9	6.35	0.82	5.69e-03	1.28e-06
CO	2169.8	13.29	1.93	1.75e-02	6.12e-06	2173.9	14.35	1.92	1.77e-02	6.01e-06	2137.6	14.62	1.91	1.81e-02	6.11e-06
CsBr	149.7	0.37	0.04	1.24e-04	8.38e-07	145.6	0.49	0.03	1.33e-04	8.03e-09	147.9	0.50	0.04	1.34e-04	8.05e-09
CsCl	214.2	0.73	0.07	3.38e-04	3.27e-08	210.7	0.96	0.07	3.62e-04	3.10e-08	213.2	0.98	0.07	3.64e-04	3.12e-08
CsF	352.6	1.61	0.18	1.18e-03	2.02e-07	356.2	2.16	0.18	1.25e-03	1.81e-07	354.3	2.17	0.18	1.27e-03	1.83e-07
CsI	119.2	0.25	0.02	6.83e-05	3.71e-07	115.6	0.33	0.02	7.36e-05	3.58e-09	117.7	0.34	0.02	7.41e-05	3.58e-09
Cl_2	559.7	2.67	0.24	1.49e-03	1.86e-07	550.0	3.15	0.24	1.50e-03	1.79e-07	580.5	2.73	0.24	1.38e-03	1.70e-07
ClF	786.1	6.16	0.52	4.36e-03	8.77e-07	782.1	5.87	0.51	4.37e-03	8.57e-07	807.8	5.09	0.51	4.01e-03	8.25e-07
ClO	853.8	5.50	0.62	5.80e-03	1.33e-06	845.0	7.02	0.61	5.99e-03	1.26e-06	801.1	4.36	0.63	5.86e-03	1.54e-06
CN	2068.6	13.09	1.90	1.74e-02	6.40e-06	2082.8	14.20	1.89	1.75e-02	6.27e-06	1849.5	27.64	1.85	2.74e-02	7.45e-06
C_2	1854.7	13.34	1.82	1.76e-02	6.92e-06	1878.7	13.87	1.81	1.75e-02	6.77e-06	1908.6	13.10	1.79	1.59e-02	6.27e-06
Li_2	351.4	2.61	0.67	7.04e-03	9.87e-06	347.4	2.53	0.68	7.11e-03	1.03e-05	342.7	2.04	0.65	6.25e-03	9.39e-06
S_2	725.6	2.84	0.30	1.57e-03	1.90e-07	720.9	3.15	0.29	1.57e-03	1.86e-07	698.7	3.80	0.29	1.75e-03	1.95e-07
F_2	916.6	11.24	0.89	1.38e-02	3.30e-05	927.1	13.63	0.89	1.29e-02	3.26e-06	1011.2	10.09	0.91	1.04e-02	2.93e-06
H_2	4401.2	121.34		3.06e+00	4.71e-02	4403.2	146.94	60.61	3.36e+00	4.59e-02	4521.1	139.28	61.52	3.12e+00	4.56e-02
HBr	2649.0	45.22	8.46	2.33e-01	3.46e-04	2728.8	60.02	8.57	2.55e-01	3.38e-04	2796.5	56.19	8.66	2.44e-01	3.32e-04
HCl	2990.9	52.82	10.59	3.07e-01	5.32e-04	3010.0	64.10	10.59	3.20e-01	5.24e-04	3062.2	60.44	10.65	3.07e-01	5.16e-04
HF	4138.3	89.88	20.96	7.98e-01	2.15e-03	4145.0	109.17	20.85	8.20e-01	2.11e-03	4142.2	106.40	20.81	8.08e-01	2.10e-03
HI	2309.0	39.64	6.43	1.69e-01	2.07e-04	2356.3	47.81	6.54	1.74e-01	2.01e-04	2429.3	43.05	6.62	1.62e-01	1.96e-04
OH	3737.8	84.88	18.91	7.24e-01	1.94e-03	3751.3	102.11	18.90	7.58e-01	1.92e-03	3822.6	96.03	19.04	7.24e-01	1.89e-03
OH^-	3700.0					3760.8	113.41	19.12	8.15e-01	1.98e-03	3825.8	91.63	19.13	7.24e-01	1.91e-03
I_2	214.5	0.61	0.04	1.14e-04	4.25e-09	217.5	0.61	0.04	1.04e-04	4.18e-09	231.2	0.53	0.04	9.53e-05	3.94e-09
IBr	268.6	0.81	0.06	1.97e-04	1.02e-07	273.2	0.89	0.06	1.88e-04	9.46e-09	289.3	0.78	0.06	1.73e-04	8.97e-09
ICl	384.3	1.50	0.11	5.35e-04	4.03e-08	386.7	1.71	0.11	5.24e-04	3.79e-08	407.3	1.51	0.11	4.86e-04	3.61e-08
IF	610.2	3.12	0.28	1.87e-03	2.37e-07	629.1	3.73	0.28	1.85e-03	2.15e-07	640.3	3.40	0.28	1.75e-03	2.10e-07
IO	681.5	4.29	0.34	2.70e-03	3.60e-07	678.2	5.36	0.33	2.75e-03	3.21e-07	611.1	2.76	0.33	1.53e-03	3.87e-07

Compound	ω_e	$\omega_e x_e$	B_e	α_e	D_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e
LiBr	563.2	3.53	0.56	5.64e-03	2.16e-06	574.2	4.59	0.55	5.96e-03	2.07e-06	575.6	4.61	0.56	5.97e-03	2.07e-06
LiCl	643.3	4.50	0.71	8.01e-03	3.41e-06	643.5	5.56	0.70	8.40e-03	3.33e-06	643.1	5.57	0.70	8.42e-03	3.32e-06
LiF	910.3	7.93	1.35	2.03e-02	1.18e-05	903.1	9.98	1.32	2.06e-02	1.13e-05	892.4	9.83	1.31	2.06e-02	1.13e-05
LiH	1405.5	23.18	7.51	2.16e-01	8.62e-04	1403.9	26.11	7.52	2.25e-01	8.65e-04	1431.2	24.53	7.57	2.11e-01	8.46e-04
LiI	498.2	3.39	0.44	4.09e-03	1.45e-06	500.8	3.55	0.44	4.22e-03	1.35e-06	501.6	3.55	0.44	4.21e-03	1.35e-06
LiO	851.5	12.50	1.20	1.51e-02		861.9	10.62	1.36	2.12e-02	1.35e-05	818.5	10.32	1.20	1.31e-02	1.03e-05
MgO	785.1	5.18	0.57	5.00e-03	1.22e-06	792.8	8.79	0.58	6.46e-03	1.21e-06	999.6	2.56	0.58	1.02e-03	7.89e-07
MgS	528.7	2.70	0.27	1.76e-03	2.76e-07	536.9	3.05	0.26	1.70e-03	2.57e-07	568.0	1.94	0.27	1.30e-03	2.36e-07
NO	1904.2	14.07	1.67	1.71e-02	5.40e-06	1916.3	15.10	1.70	1.76e-02	5.37e-06	1922.7	11.61	1.69	1.54e-02	5.25e-06
NO^+	2376.4	16.26	2.00	1.89e-02	5.64e-06	2387.3	17.38	1.99	1.89e-02	5.54e-06	2191.3	23.00	1.94	2.34e-02	6.12e-06
NS	1218.7	7.28	0.77	6.35e-03	1.20e-06	1213.7	8.27	0.76	6.30e-03	1.20e-06	1455.1	17.66	0.79	6.01e-03	9.29e-07
N_2	2358.6	14.32	2.00	1.73e-02	5.76e-06	2370.3	15.13	1.99	1.74e-02	5.61e-06	2221.1	20.38	1.95	2.10e-02	6.06e-06
N_2^+	2207.0	16.10	1.93	1.88e-02	6.10e-06	2221.3	17.18	1.93	1.90e-02	5.79e-06	2055.8	20.22	1.87	2.13e-02	6.17e-06
O_2	1580.2	11.98	1.44	1.59e-02	4.84e-06	1596.0	12.94	1.44	1.58e-02	4.73e-06	1282.3	24.22	1.36	2.46e-02	6.06e-06
PN	1337.2	6.98	0.79	5.54e-03	1.09e-06	1329.7	7.43	0.77	5.52e-03	1.05e-06	1194.2	11.27	0.75	7.32e-03	1.20e-06
PF	846.8	4.49	0.57	4.56e-03		842.3	5.52	0.56	4.71e-03	9.68e-07	846.0	5.35	0.56	4.64e-03	9.60e-07
PO	1233.3	6.56	0.73	5.50e-03	1.30e-06	1220.8	7.31	0.72	5.49e-03	9.96e-07	1194.3	6.86	0.71	5.45e-03	1.01e-06
KBr	213.0	0.80	0.08	4.00e-04		215.1	0.92	0.08	4.10e-04	4.12e-08	216.9	0.94	0.08	4.13e-04	4.14e-08
KCl	281.0	1.30	0.13	7.90e-04	1.09e-07	272.9	1.41	0.12	7.92e-04	1.01e-07	274.5	1.44	0.12	7.97e-04	1.02e-07
KF	428.0	2.40	0.28	2.34e-03	4.83e-07	411.6	2.80	0.27	2.35e-03	4.57e-07	408.0	2.76	0.27	2.36e-03	4.62e-07
KI	186.5	0.57	0.06	2.68e-04	2.89e-07	183.7	0.72	0.06	2.76e-04	2.40e-08	185.6	0.73	0.06	2.78e-04	2.41e-08
RbBr	169.5	0.46	0.05	1.86e-04		167.9	0.60	0.05	1.90e-04	1.32e-08	168.7	0.60	0.05	1.91e-04	1.33e-08
RbCl	228.0	0.92	0.09	4.54e-04	4.95e-08	232.0	1.10	0.08	4.60e-04	4.34e-08	232.5	1.11	0.08	4.63e-04	4.36e-08
RbF	376.0	1.90	0.21	1.52e-03	2.68e-07	369.9	2.34	0.20	1.51e-03	2.25e-07	365.3	2.32	0.20	1.52e-03	2.27e-07
RbI	138.5	0.34	0.03	1.09e-04	7.38e-09	136.8	0.42	0.03	1.13e-04	6.66e-09	137.7	0.43	0.03	1.13e-04	6.68e-09
NaBr	302.1	1.50	0.15	9.41e-04	1.55e-07	291.5	1.65	0.15	1.13e-03	1.58e-07	293.4	1.70	0.15	1.13e-03	1.56e-07
NaCl	366.0	2.05	0.22	6.25e-03	3.12e-07	354.8	3.29	0.22	2.13e-03	3.24e-07	355.0	3.26	0.22	2.11e-03	3.21e-07
NaF	536.0	3.40	0.44	4.56e-03	1.16e-06	524.5	5.58	0.43	5.36e-03	1.20e-06	517.2	5.42	0.43	5.32e-03	1.20e-06
NaH	1176.0	21.20	4.89	1.31e-01	3.32e-04	1163.0	25.37	4.94	1.06e-01	3.56e-04	1191.8	23.15	4.96	9.67e-02	3.43e-04
NaI	258.0	1.08	0.12	6.48e-04	9.73e-08	248.3	0.69	0.11	5.30e-04	9.81e-08	248.4	0.71	0.11	5.52e-04	9.85e-08
SH	2711.6	59.90	9.46	2.70e-01	4.80e-04	2707.0	59.34	9.59	2.95e-01	4.82e-04	2781.9	54.08	9.69	2.77e-01	4.70e-04
SF	837.6	4.47	0.56	4.59e-03	9.75e-07	836.3	5.42	0.55	4.47e-03	9.27e-07	850.0	5.16	0.55	4.36e-03	9.11e-07
SO	1149.2	5.63	0.72	5.74e-03	1.13e-06	1138.4	7.13	0.70	5.71e-03	1.08e-06	1074.9	-1.73	0.69	4.65e-03	1.13e-06

Table S5 Percent deviation for Vibrational harmonic frequency ω_e, First anharmonic correction $\omega_e x_e$, Equilibrium rotational constant B_e, First correction of the rotational constant α_e, Centrifugal distortion constant D_e, for different methods and analytical potentials fitted on CCSD(T) without energy threshold, from the reference indicated below.

Reference:	Experiment					CCSD(T)				
Method	ω_e	$\omega_e x_e$	B_e	α_e	D_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e
CCSD(T)	2.92	28.07	2.76	14.64	26.91					
MP2	6.59	40.35	2.46	21.09	28.19	6.25	27.84	2.14	18.30	9.39
Sun	2.96	27.38	2.76	14.48	26.92	0.05	1.01	0.01	0.39	0.10
Hulburt-Hirschfelder	2.94	26.86	2.76	14.18	26.91	0.06	1.84	0.02	0.75	0.12
Wei-Hua	2.89	26.19	2.76	14.01	26.91	0.10	4.93	0.06	2.23	0.18
Tietz-II	2.87	26.14	2.76	13.93	26.90	0.13	4.87	0.06	2.31	0.29
Rafi	2.86	25.89	2.77	13.59	26.90	0.20	3.15	0.05	2.75	0.49
Levine	2.88	26.20	2.76	14.07	26.92	0.28	6.78	0.07	4.78	0.63
Murrell-Sorbie	2.98	30.48	2.75	14.42	26.97	0.45	5.90	0.05	2.09	0.80
Cahill	3.02	30.07	2.75	14.29	26.99	0.48	4.61	0.03	1.69	0.89
Deng-Fan	2.93	28.22	2.77	16.69	26.93	0.56	12.63	0.13	9.74	1.08
Morse	2.91	30.79	2.73	12.31	27.01	0.69	11.87	0.09	3.68	1.21
Frost-Musulin	2.88	28.19	2.75	12.40	26.99	0.71	10.52	0.09	3.93	1.31
Poschl-Teller	2.88	28.93	2.74	12.24	27.01	0.76	10.78	0.09	3.97	1.39
Linnett	2.90	28.47	2.74	12.72	26.96	0.77	11.87	0.10	4.24	1.39
Tietz-I	3.07	23.69	2.87	15.24	26.91	0.79	16.21	0.37	9.14	1.81
Rydberg	2.91	32.90	2.71	12.09	27.07	0.85	12.85	0.10	3.86	1.49
Valence-State	3.06	23.01	2.80	13.67	26.80	0.87	11.26	0.10	4.41	1.61
Varshni	2.90	33.90	2.70	13.34	27.13	1.03	13.40	0.12	6.25	1.83
Rosen-Morse	2.93	33.28	2.71	11.75	27.11	1.06	13.22	0.10	4.36	1.90
Tang2003a	2.83	31.81	2.75	17.70	27.10	1.07	17.72	0.42	15.43	2.42
Pseudo-Gaussian	2.95	35.71	2.68	11.76	27.21	1.23	14.29	0.12	4.56	2.15
Noorizadeh	2.99	40.61	2.99	30.54	27.23	1.30	36.89	1.03	30.52	3.58
Kratzer	2.39	60.84	4.10	49.58	27.73	1.91	65.99	1.95	51.67	5.65
Buckingham	3.67	65.22	2.86	27.03	27.04	2.15	49.12	0.40	24.64	3.85
Wang-Buckingham	3.93	65.38	2.55	13.59	27.81	2.98	40.75	0.28	10.46	5.05
Lippincott	2.26	95.12	5.49	99.75	29.70	3.02	95.84	3.66	99.75	11.34
Harmonic	3.48	-	-	-	-	4.87	-	-	-	-
Xie2005a	3.60	87.68	5.68	100	31.91	5.02	89.16	3.89	100	16.11
Lennard-Jones	16.84	100	7.34	100	77.03	16.09	100	7.71	100	55.95

Table S6 Percent deviation for Vibrational harmonic frequency ω_e, First anharmonic correction $\omega_e x_e$, Equilibrium rotational constant B_e, First correction of the rotational constant α_e, Centrifugal distortion constant D_e, for different methods and analytical potentials fitted on CCSD(T) with an energy threshold of 5000 cm^{-1}, from the reference indicated below.

Reference:	Experiment					CCSD(T)				
Method	ω_e	$\omega_e x_e$	B_e	α_e	D_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e
CCSD(T)	2.91	24.90	2.77	13.76	26.94					
MP2	6.60	39.61	2.46	19.96	28.20	6.27	31.04	2.14	18.26	9.36
Sun	2.92	24.75	2.76	13.84	26.95	0.02	0.27	0.00	0.25	0.05
Hulburt-Hirschfelder	2.95	23.79	2.77	13.48	26.96	0.08	1.58	0.01	0.56	0.13
Tietz-II	2.94	22.55	2.77	12.96	26.95	0.11	3.68	0.05	2.08	0.18
Cahill	2.93	25.08	2.75	13.26	26.96	0.18	2.21	0.02	1.70	0.37
Wei-Hua	3.05	22.07	2.78	12.87	26.99	0.23	5.44	0.05	2.10	0.37
Murrell-Sorbie	2.96	26.34	2.76	13.60	26.99	0.31	4.52	0.03	2.48	0.61
Levine	3.01	22.28	2.77	12.87	27.00	0.32	6.68	0.05	3.07	0.63
Deng-Fan	2.90	25.67	2.77	16.52	26.98	0.38	9.49	0.11	9.71	0.88
Tietz-I	3.01	20.83	2.77	13.42	26.94	0.47	8.54	0.07	5.05	1.01
Morse	2.88	25.57	2.76	12.10	27.02	0.48	7.19	0.05	3.91	0.97
Valence-State	3.01	21.90	2.77	13.56	26.92	0.52	6.92	0.05	4.38	1.08
Frost-Musulin	2.87	24.17	2.76	12.33	27.02	0.52	6.41	0.05	3.83	1.07
Poschl-Teller	2.87	24.55	2.76	12.22	27.03	0.56	6.57	0.05	3.96	1.13
Rydberg	2.86	26.47	2.75	11.95	27.05	0.56	7.75	0.05	4.42	1.14
Linnett	2.90	28.22	2.75	12.30	27.00	0.62	12.11	0.05	3.90	1.20
Varshni	2.83	26.42	2.76	13.37	27.08	0.64	8.19	0.08	6.86	1.33
Rosen-Morse	2.88	27.42	2.75	11.91	27.08	0.73	8.74	0.05	4.76	1.46
Pseudo-Gaussian	2.83	27.00	2.76	12.01	27.11	0.74	8.05	0.06	5.80	1.51
Tang2003a	2.83	26.57	2.74	16.86	27.01	0.85	14.81	0.25	15.07	1.45
Rafi	3.25	25.14	2.79	18.82	27.04	0.90	12.07	0.33	13.78	0.96
Buckingham	3.25	62.56	2.80	26.11	27.10	1.58	45.62	0.33	24.48	2.99
Noorizadeh	3.35	42.76	2.80	34.92	27.02	1.89	40.76	0.64	34.38	2.43
Wang-Buckingham	3.24	52.11	2.70	16.15	27.48	1.95	32.96	0.12	14.45	3.81
Lippincott	3.71	74.28	4.40	100	28.46	2.09	67.01	2.34	100	7.40
Kratzer	3.87	59.90	3.63	49.84	26.85	2.55	64.11	1.29	50.18	2.80
Xie2005a	5.39	86.94	4.48	100	27.11	4.86	88.49	2.41	100	6.59
Harmonic	5.65	-	-	-	-	5.07	-	-	-	-
Lennard-Jones	15.25	100	4.89	100	30.34	14.96	100	5.19	100	12.46

Table S7 Percent deviation for Vibrational harmonic frequency ω_e, First anharmonic correction $\omega_e x_e$, Equilibrium rotational constant B_e, First correction of the rotational constant α_e, Centrifugal distortion constant D_e, for different methods and analytical potentials fitted on experimental data without energy threshold, from the reference indicated below.

Reference:	Experiment				
Method	ω_e	$\omega_e x_e$	B_e	α_e	D_e
Sun	0.38	26.76	0.68	11.88	1.45
Murrell-Sorbie	1.20	22.70	0.74	9.75	2.28
Pseudo-Gaussian	1.42	15.53	1.70	15.70	4.83
Varshni	1.38	27.24	0.96	19.22	5.12
Hulburt-Hirschfelder	1.17	21.39	0.78	9.16	1.94
Levine	1.50	19.69	0.75	10.32	3.39
Rafi	1.39	20.03	0.70	10.91	4.07
Poschl-Teller	1.86	22.48	0.74	10.29	4.07
Rydberg	1.98	18.29	1.11	14.63	7.32
Noorizadeh	1.90	19.96	0.68	8.74	4.67
Wei-Hua	1.97	26.07	0.65	8.22	3.47
Morse	2.17	22.18	0.81	11.42	5.90
Frost-Musulin	2.12	28.61	0.90	14.04	3.87
Linnett	2.18	52.00	1.97	38.93	12.20
Tietz-II	2.90	25.01	0.65	9.52	5.72
Valence-State	2.52	55.08	2.14	35.84	8.69
Lippincott	3.52	25.62	11.54	100	36.19
Cahill	3.27	85.69	1.51	43.28	7.56
Deng-Fan	3.34	59.13	2.20	38.12	7.74
Tang2003a	3.57	21.10	0.78	12.12	8.19
Tietz-I	3.44	60.27	2.26	39.74	8.08
Rosen-Morse	5.15	19.36	1.13	20.28	12.58
Buckingham	6.09	100	6.82	98.79	27.51
Kratzer	11.00	60.98	5.23	42.76	10.99
Harmonic	20.42	-	-	-	-
Xie2005a	21.28	83.07	11.31	95.59	17.33
Wang-Buckingham	26.43	70.84	2.03	43.54	26.57
Lennard-Jones	66.23	100	22.68	100	35.37

Table S8 Vibrational properties: Ground state frequency ω_e (1/cm) Anharmonic frequency $\omega_e x_e$ (1/cm) Rotational constant in equilibrium position B_e (1/cm) Rotational constant - first term α_e (1/cm) Centrifugal distortion constant D_e (1/cm) from experiment[1] or computed using Psi4[28] based on experimental data. Root Mean Square Deviation (RMSD) and Mean Signed Error (MSE) are given at the bottom.

Molecule	ω_e		$\omega_e x_e$		B_e		α_e		D_e	
	Exper	Psi4	Exper	Psi4	Exper	Psi4	Exper	Psi4	Exper	Psi4
C_2	1854.7	1880.2	13.34	14.92	1.82	1.81	1.76e-02	1.82e-02	6.92e-06	6.76e-06
CF	1308.1	1322.6	11.10	14.84	1.42	1.42	1.84e-02	2.00e-02	6.50e-06	6.49e-06
CH	2858.5	2920.8	63.02	83.63	14.46	14.73	5.34e-01	6.05e-01	1.45e-03	1.50e-03
Li_2	351.4	347.4	2.61	2.53	0.67	0.68	7.04e-03	7.11e-03	9.87e-06	1.03e-05
LiH	1405.5	1403.9	23.18	26.11	7.51	7.52	2.16e-01	2.25e-01	8.62e-04	8.65e-04
CN	2068.6	2084.7	13.09	15.69	1.90	1.90	1.74e-02	1.84e-02	6.40e-06	6.27e-06
N_2^+	2207.0	2220.7	16.10	18.47	1.93	1.93	1.88e-02	2.01e-02	6.10e-06	5.80e-06
H_2	4401.2	4403.2	121.34	146.94		60.61	3.06e+00	3.36e+00	4.71e-02	4.59e-02
HF	4138.3	4143.1	89.88	109.70	20.96	20.85	7.98e-01	8.44e-01	2.15e-03	2.11e-03
I_2	214.5	217.2	0.61	0.65	0.04	0.04	1.14e-04	1.11e-04	4.25e-09	4.19e-09
O_2	1580.2	1598.1	11.98	14.49	1.44	1.44	1.59e-02	1.67e-02	4.84e-06	4.72e-06
N_2	2358.6	2373.4	14.32	17.08	2.00	1.99	1.73e-02	1.83e-02	5.76e-06	5.60e-06
CO	2169.8	2176.6	13.29	16.14	1.93	1.92	1.75e-02	1.86e-02	6.12e-06	6.00e-06
OH	3737.8	3747.7	84.88	99.87	18.91	18.90	7.24e-01	7.76e-01	1.94e-03	1.92e-03
NO	1904.2	1919.3	14.07	17.01	1.67	1.70	1.71e-02	1.85e-02	5.40e-06	5.36e-06
RMSD		15.2		8.28		0.08		7.47e-02		2.90e-04
MSE		13.4		7.02		0.01		3.23e-02		-7.75e-05

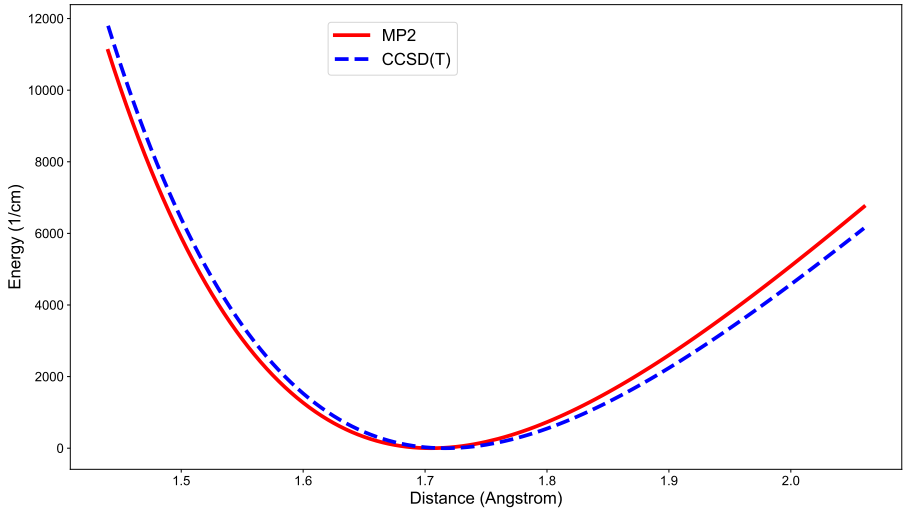

Fig. S1 Compound boron monochloride (BCl).

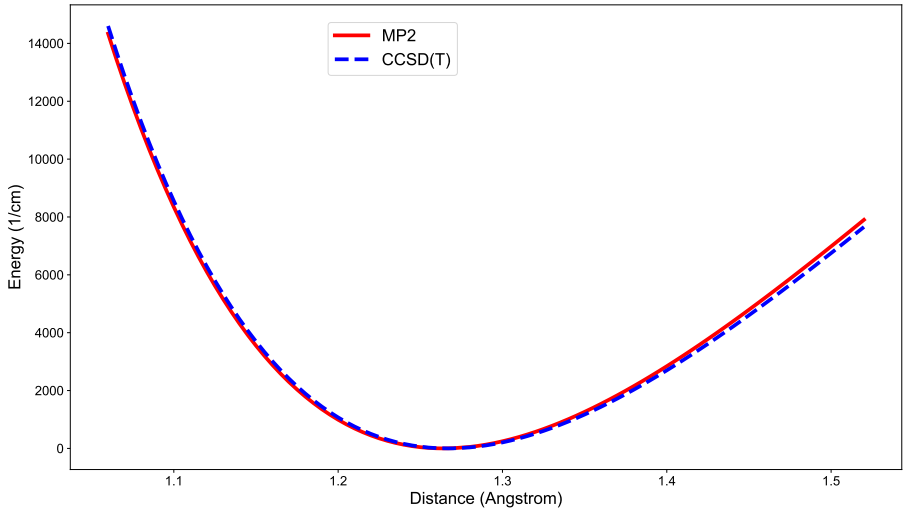

Fig. S2 Compound boron monofluoride (BF).

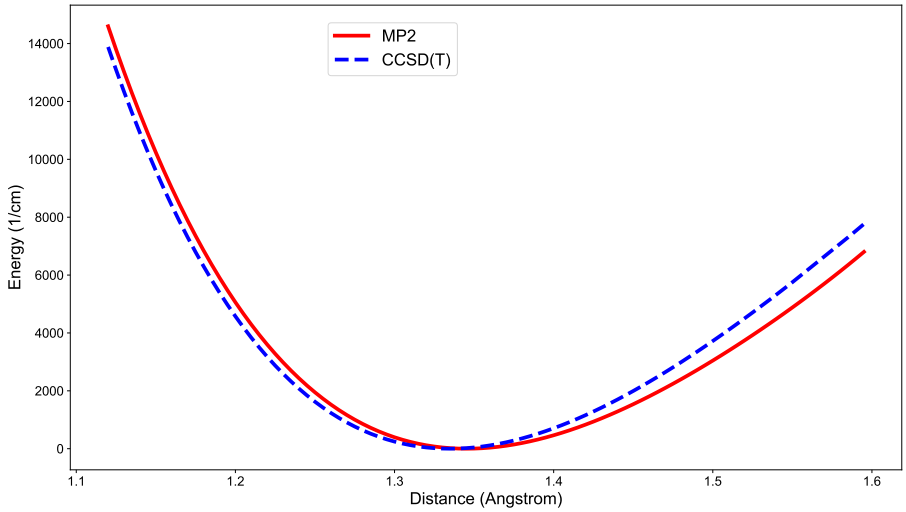

Fig. S3 Compound beryllium oxide (BeO).

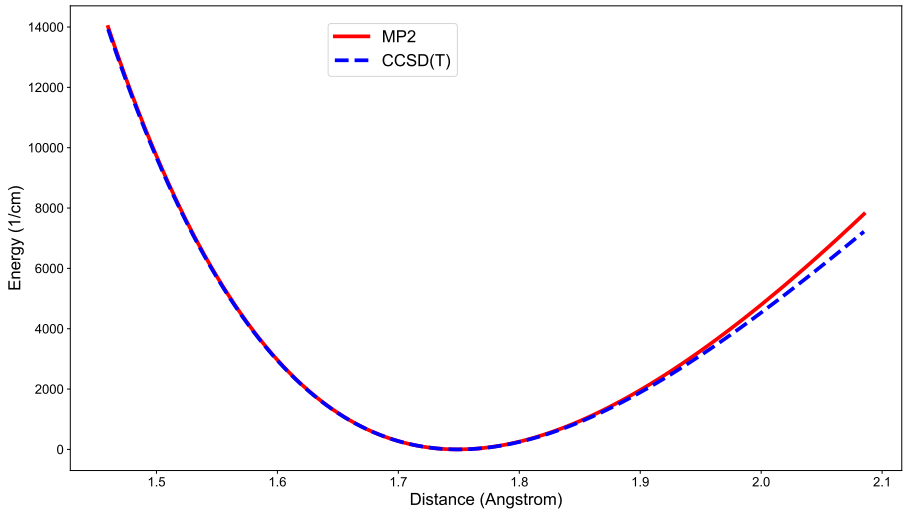

Fig. S4 Compound beryllium sulfide (BeS).

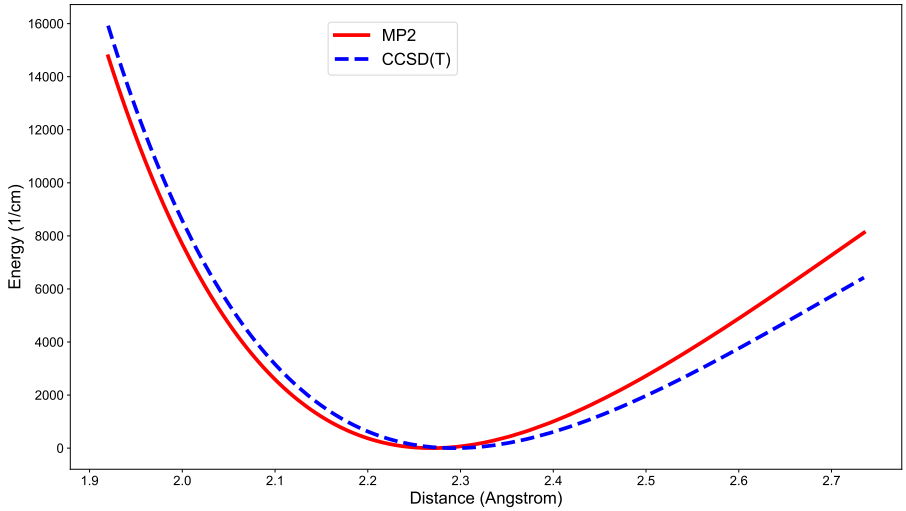

Fig. S5 Compound bromine (Br_2).

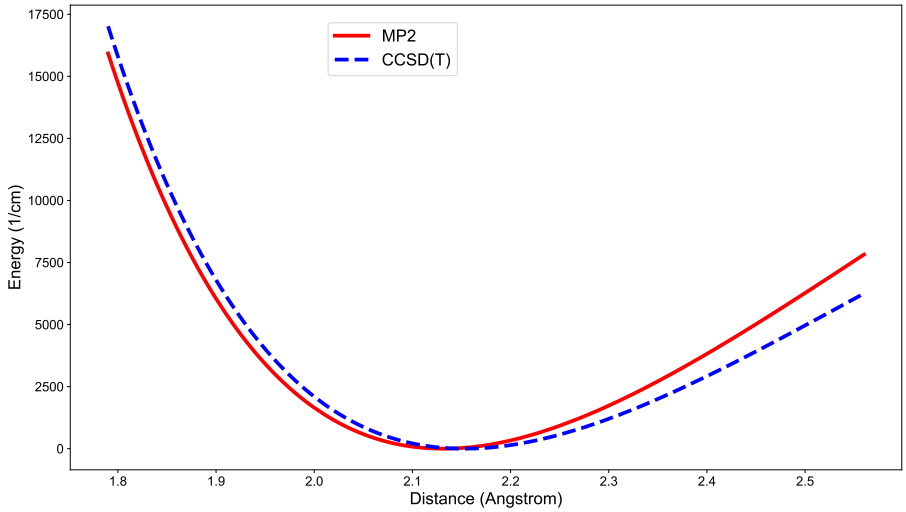

Fig. S6 Compound bromine chloride (BrCl).

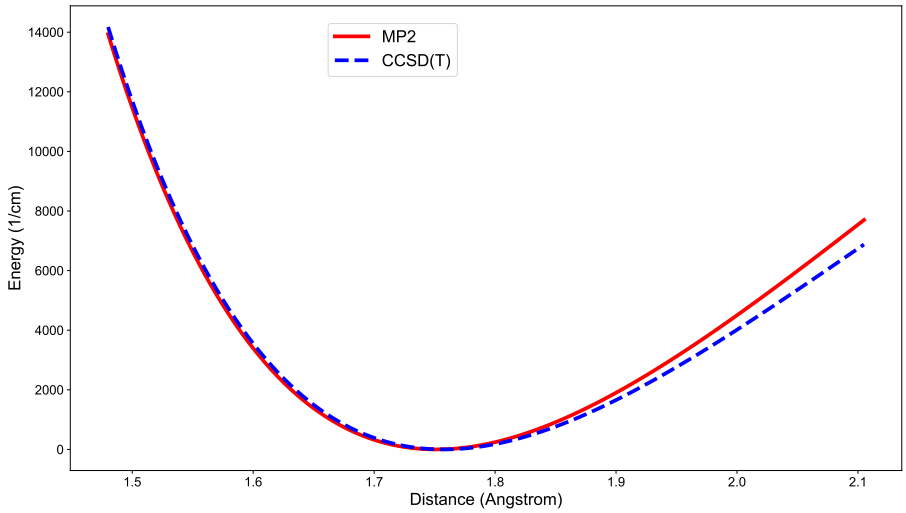

Fig. S7 Compound bromine fluoride (BrF).

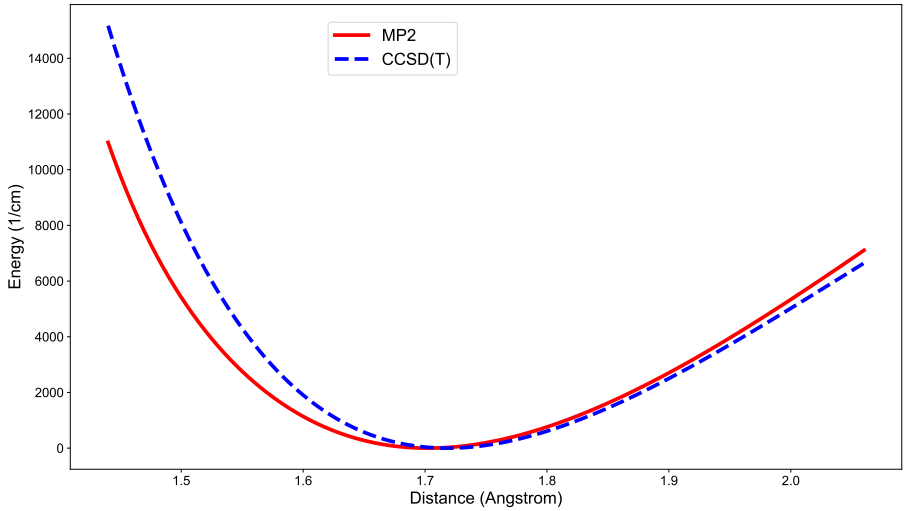

Fig. S8 Compound bromine monoxide (BrO).

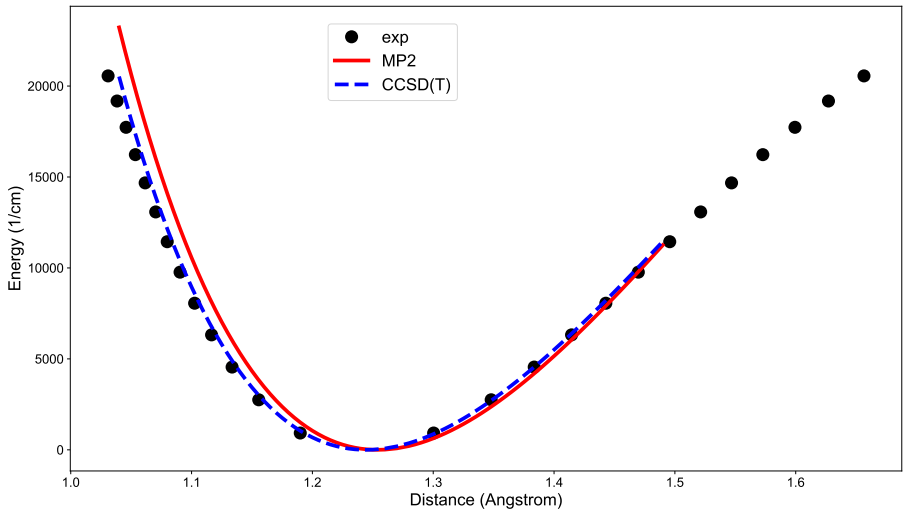

Fig. S9 Compound dicarbon (C_2). Experimental data from ref. 29.

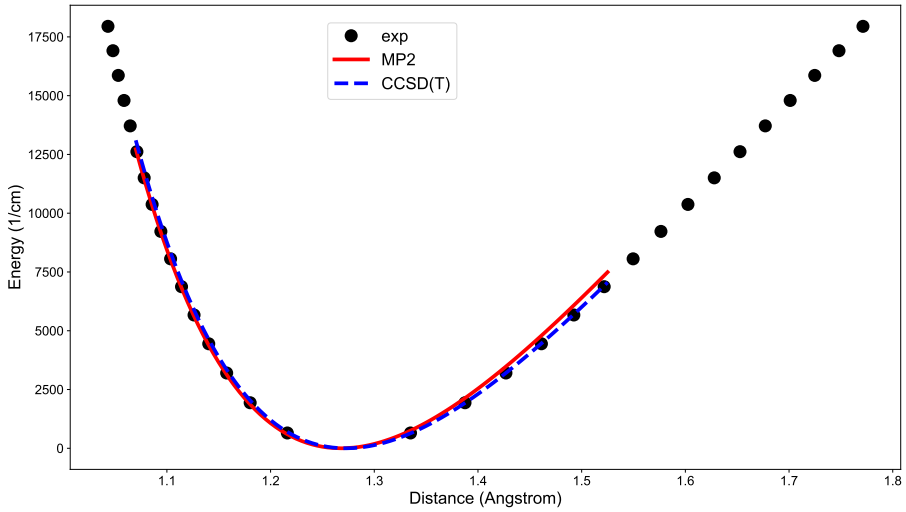

Fig. S10 Compound carbon monofluoride (CF). Experimental data from ref. 29.

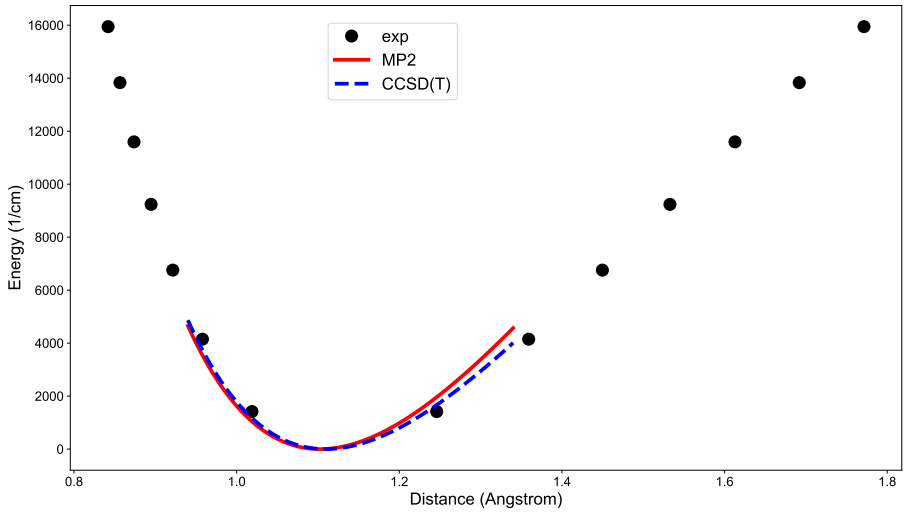

Fig. S11 Compound carbon monohydride (CH). Experimental data from ref. 29.

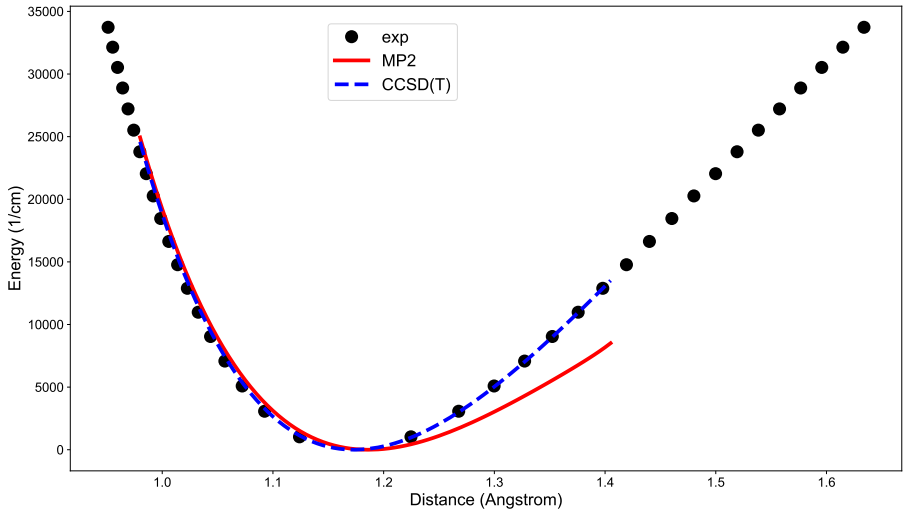

Fig. S12 Compound cyano radical (CN). Experimental data from ref. 29.

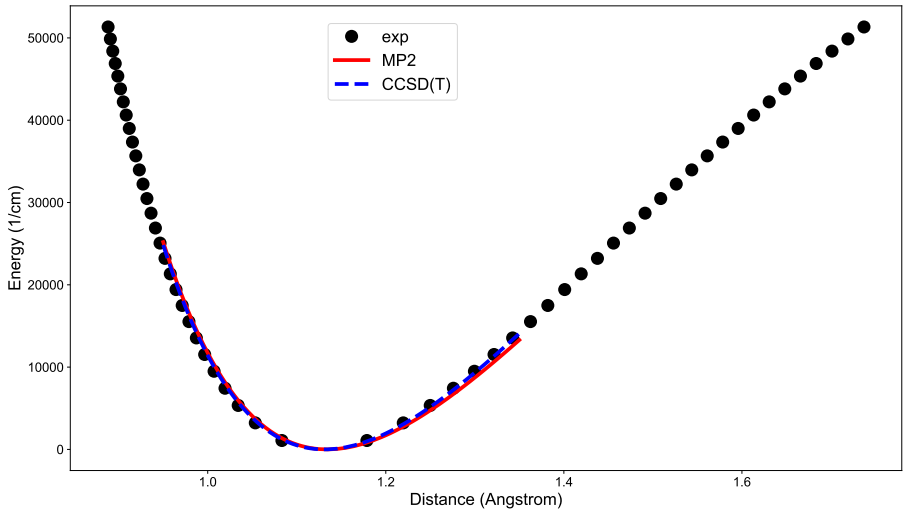

Fig. S13 Compound carbon monoxide (CO). Experimental data from ref. 30.

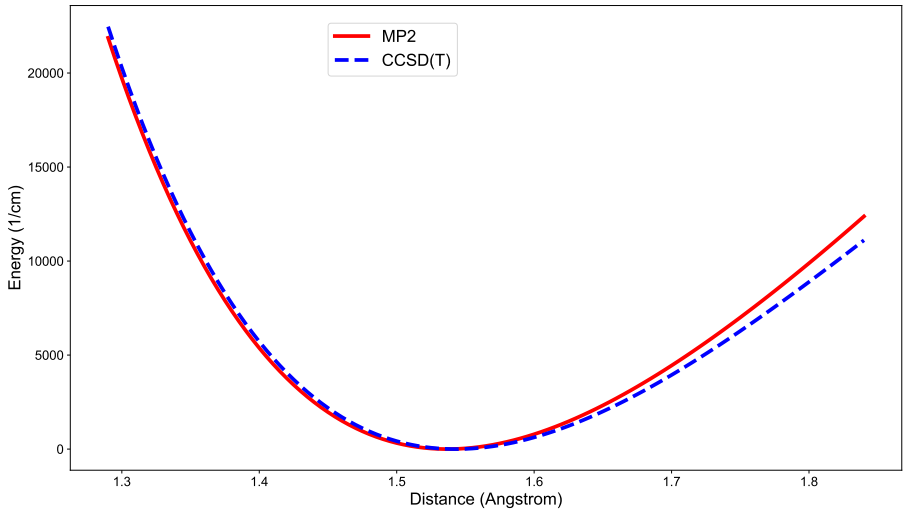

Fig. S14 Compound carbon monosulfide (CS).

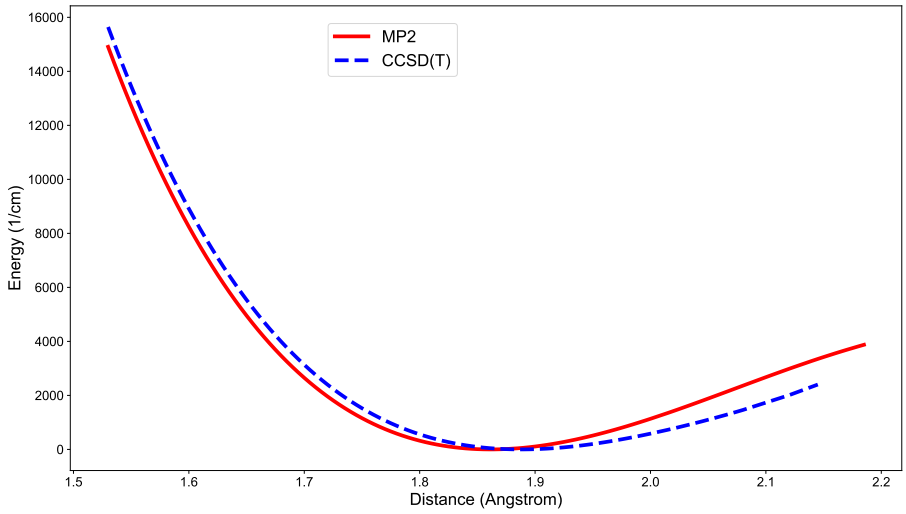

Fig. S15 Compound calcium oxide (CaO).

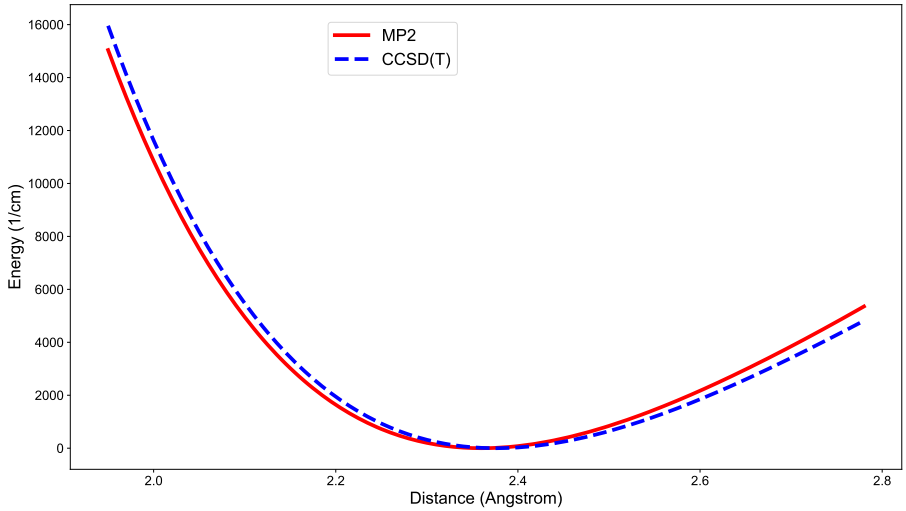

Fig. S16 Compound calcium sulfide (CaS).

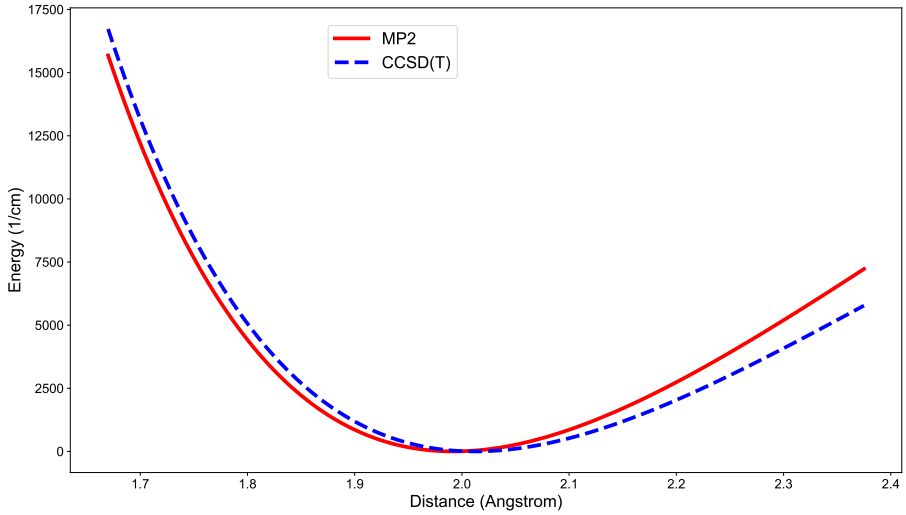

Fig. S17 Compound chlorine (Cl_2).

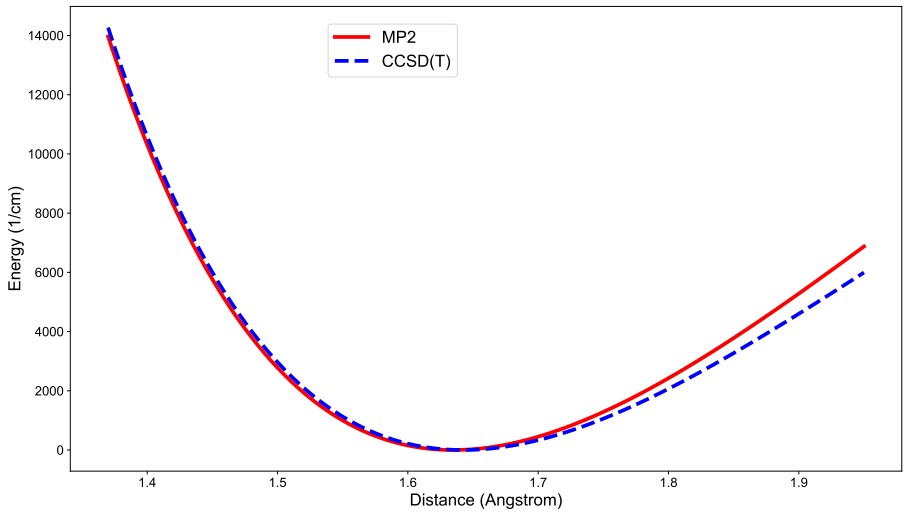

Fig. S18 Compound chlorine fluoride (ClF).

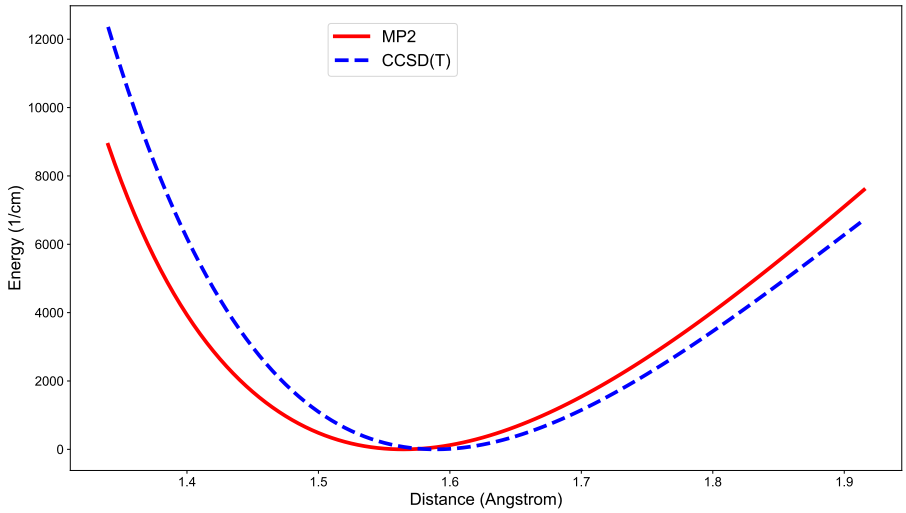

Fig. S19 Compound chlorine monoxide (ClO).

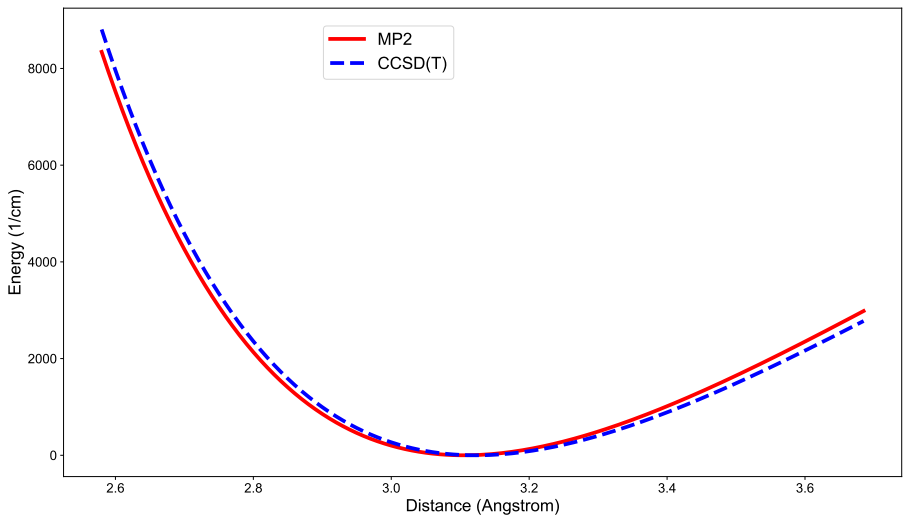

Fig. S20 Compound cesium bromide (CsBr).

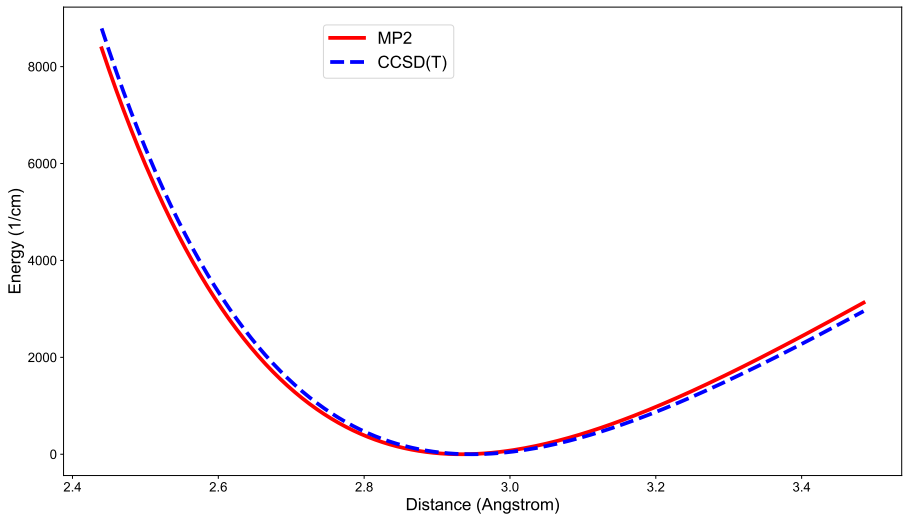

Fig. S21 Compound cesium chloride (CsCl).

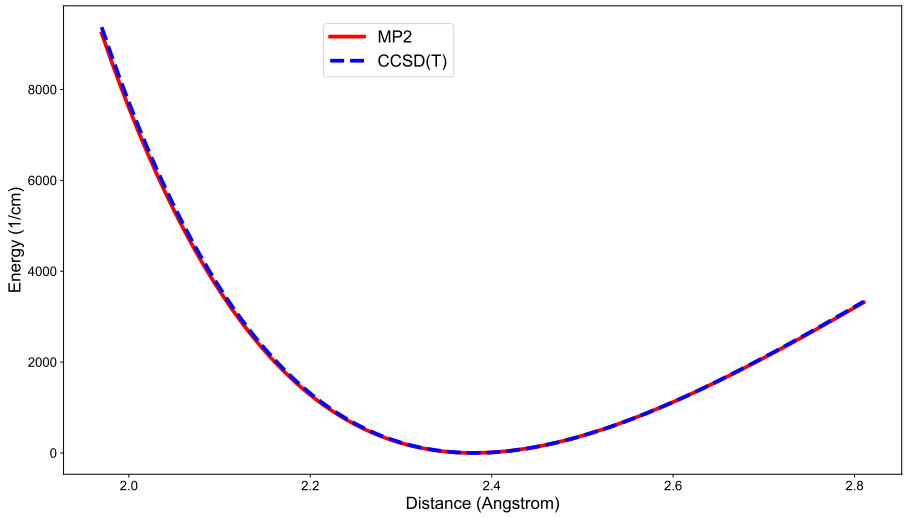

Fig. S22 Compound cesium fluoride (CsF).

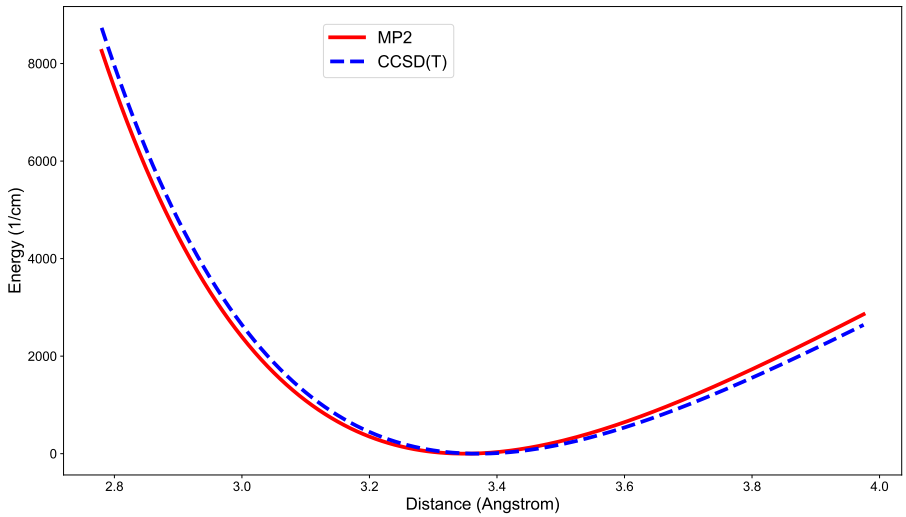

Fig. S23 Compound cesium iodide (CsI).

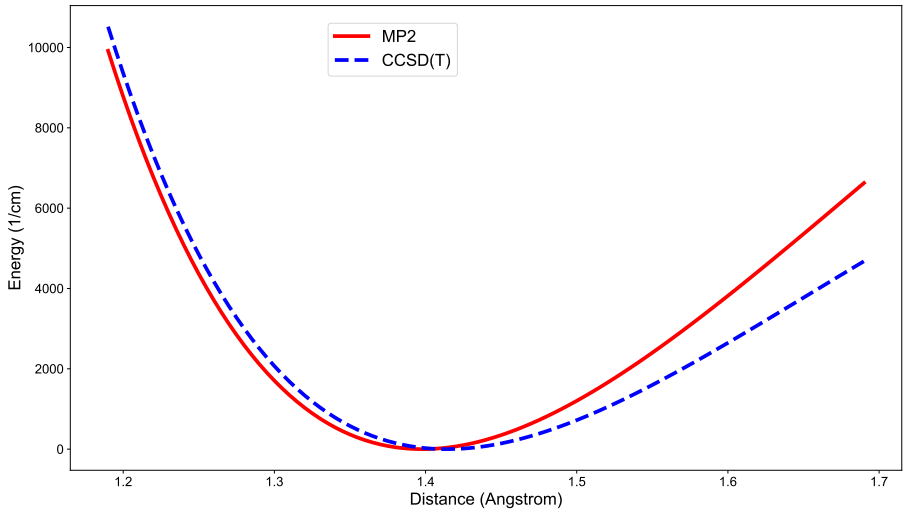

Fig. S24 Compound fluorine (F_2).

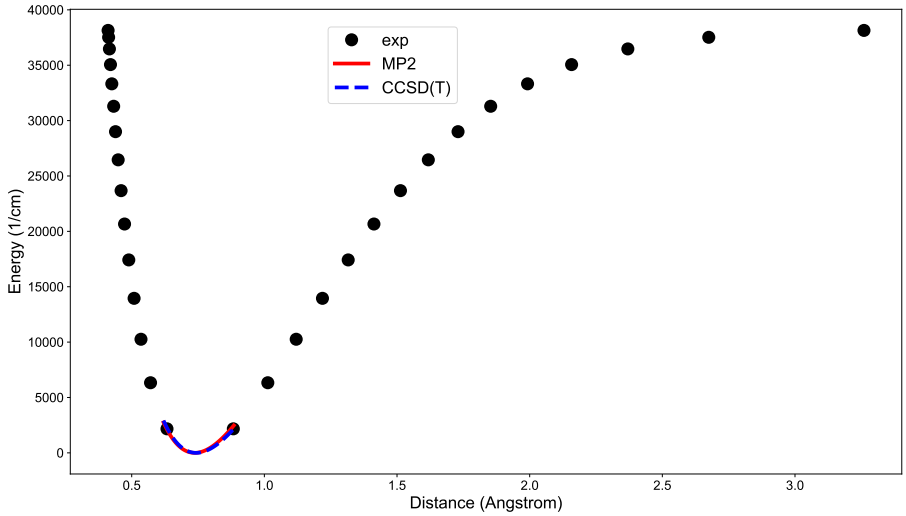

Fig. S25 Compound hydrogen (H_2). Experimental data from ref. 31.

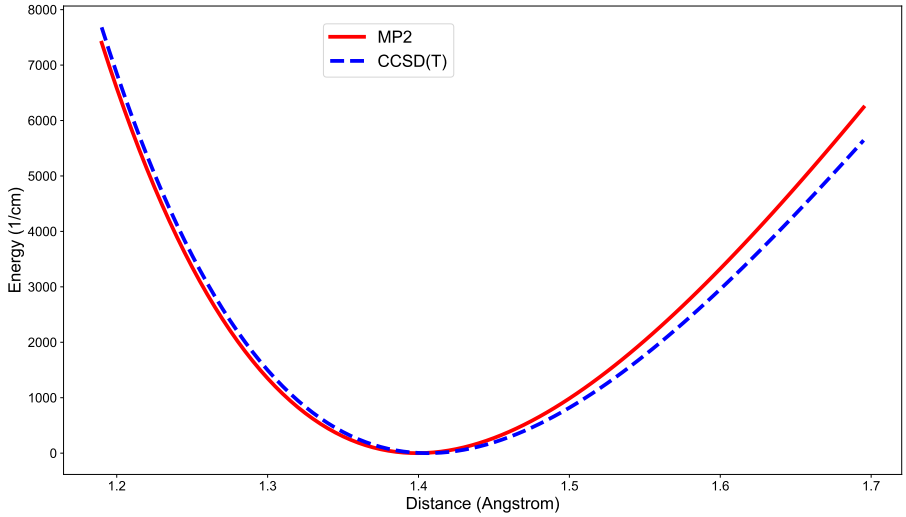

Fig. S26 Compound hydrogen bromide (HBr).

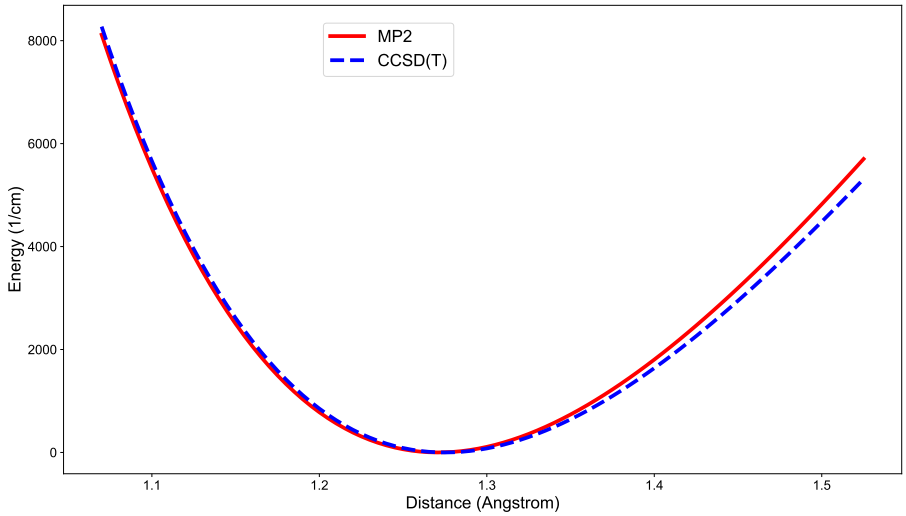

Fig. S27 Compound hydrogen chloride (HCl).

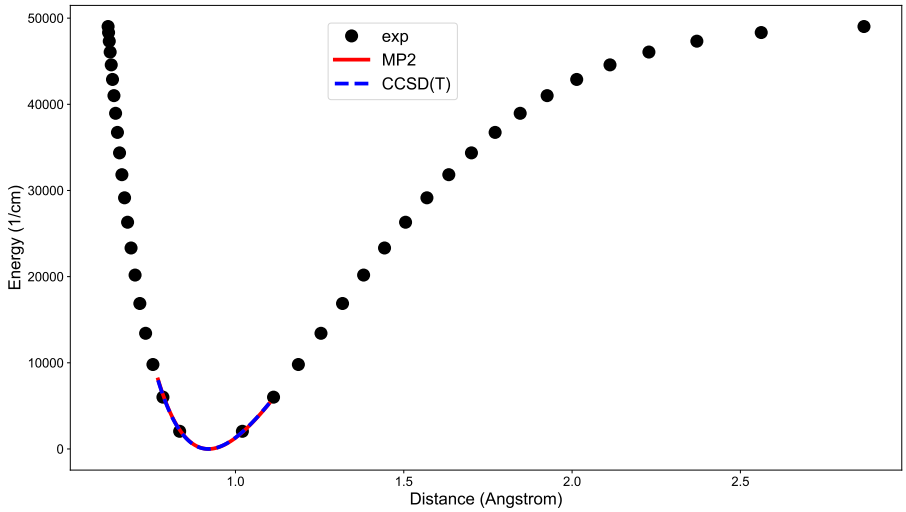

Fig. S28 Compound hydrogen fluoride (HF). Experimental data from ref. 32.

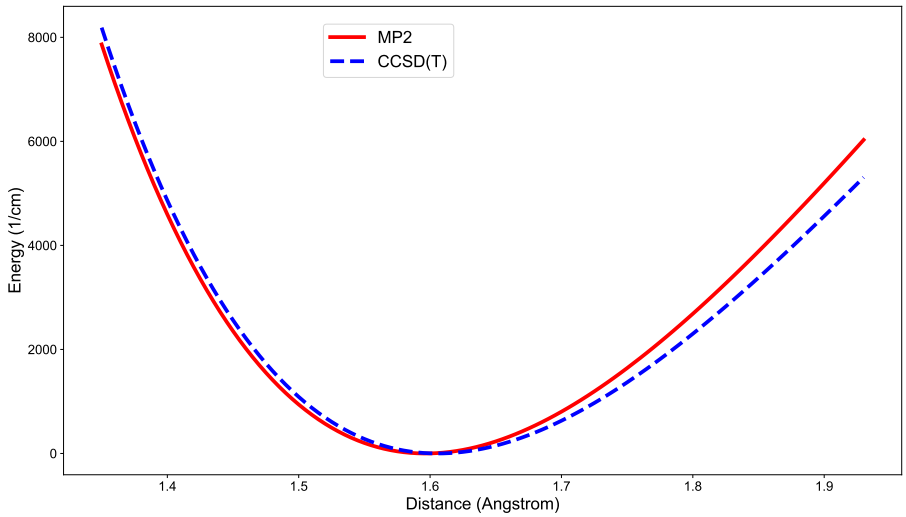

Fig. S29 Compound hydrogen iodide (HI).

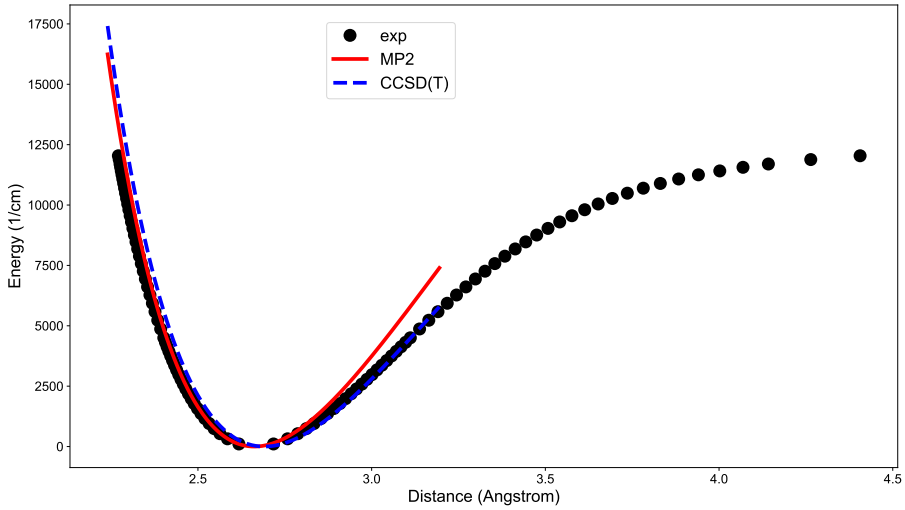

Fig. S30 Compound iodine (I_2). Experimental data from ref. 31.

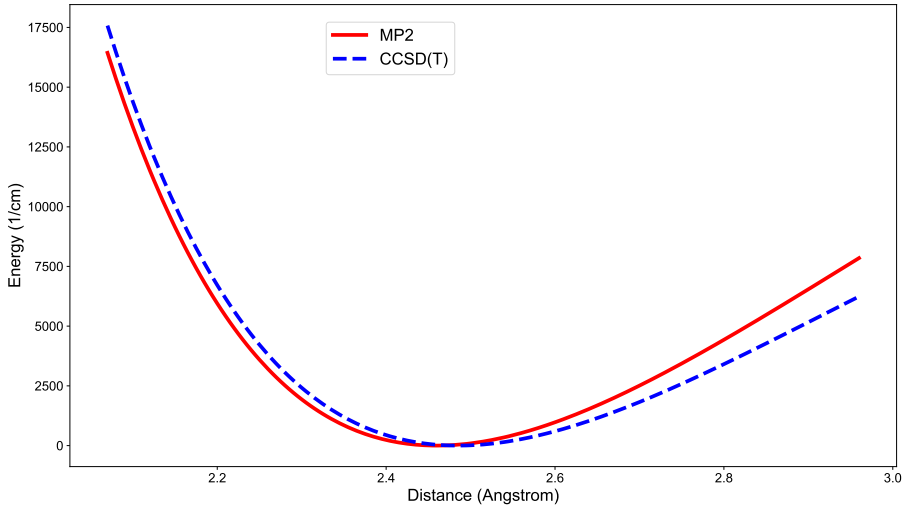

Fig. S31 Compound iodine bromide (IBr).

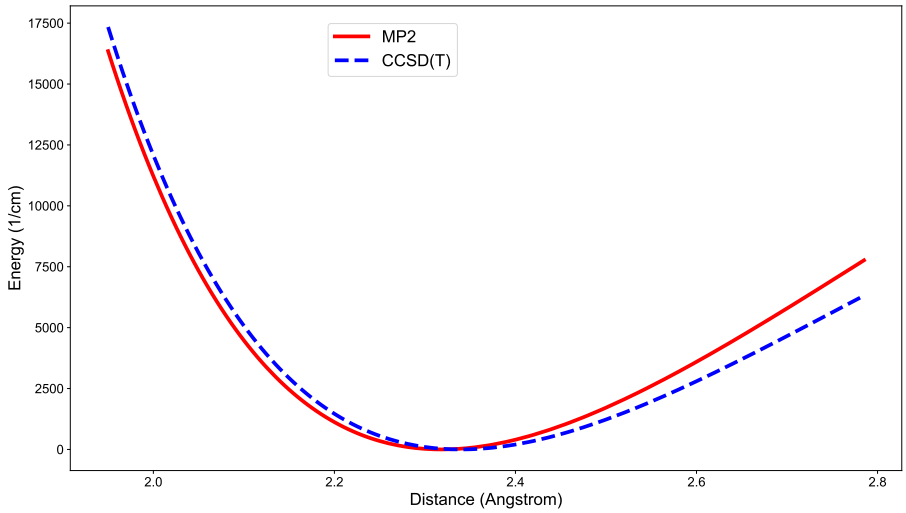

Fig. S32 Compound iodine chloride (ICl).

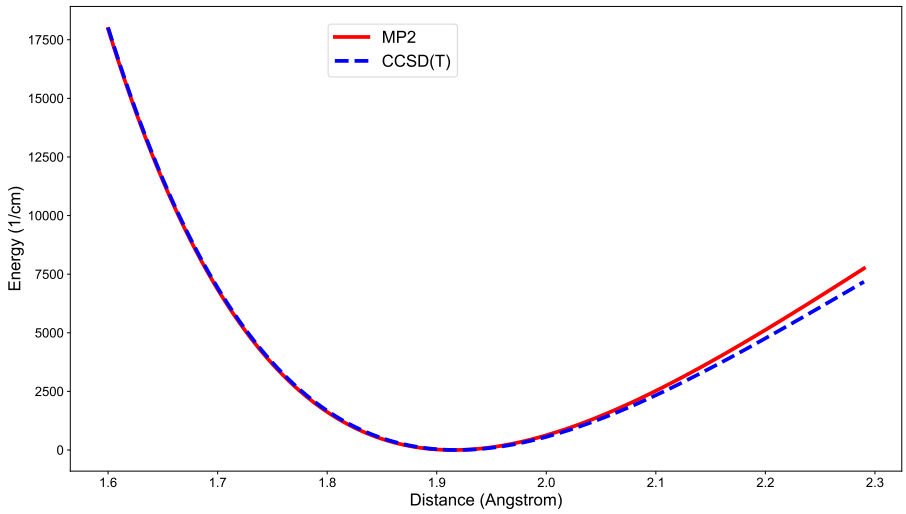

Fig. S33 Compound iodine fluoride (IF).

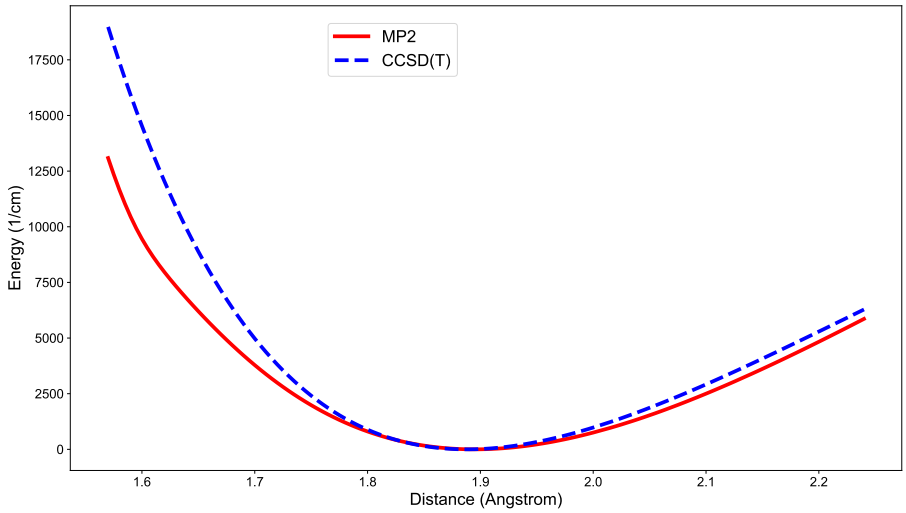

Fig. S34 Compound iodine monoxide (IO).

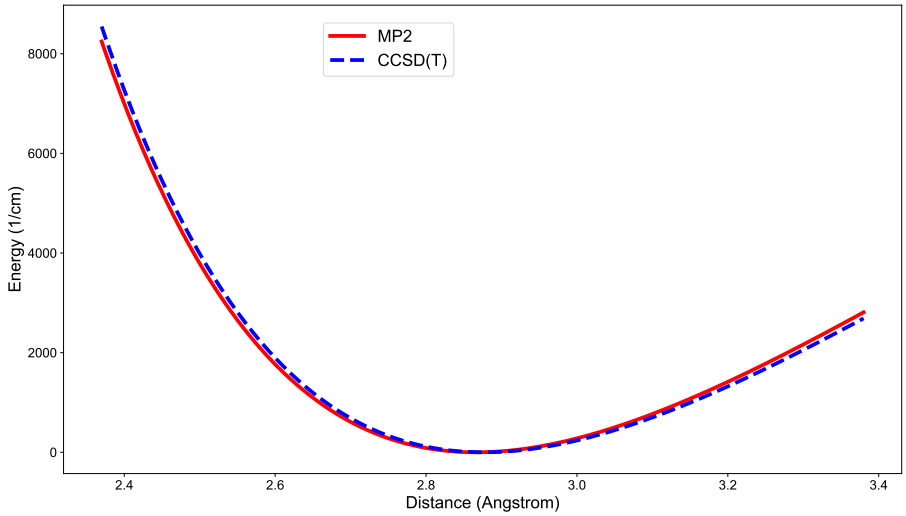

Fig. S35 Compound potassium bromide (KBr).

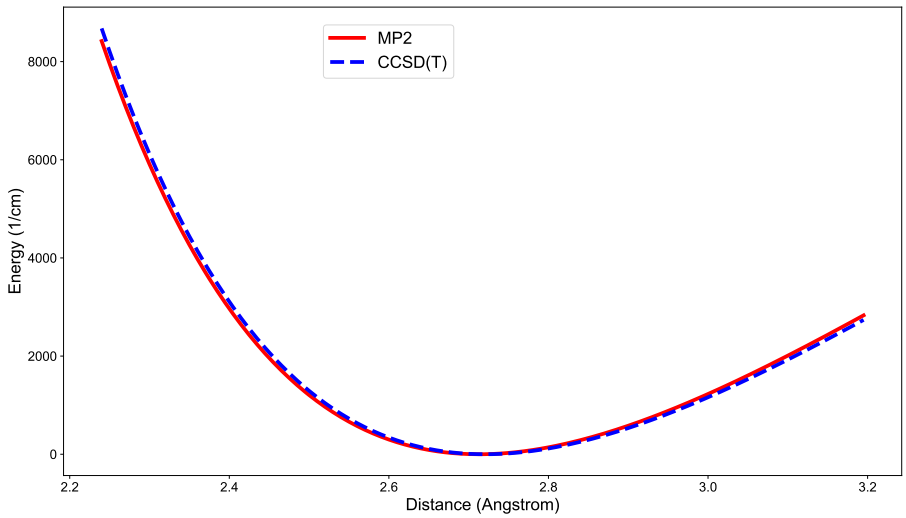

Fig. S36 Compound potassium chloride (KCl).

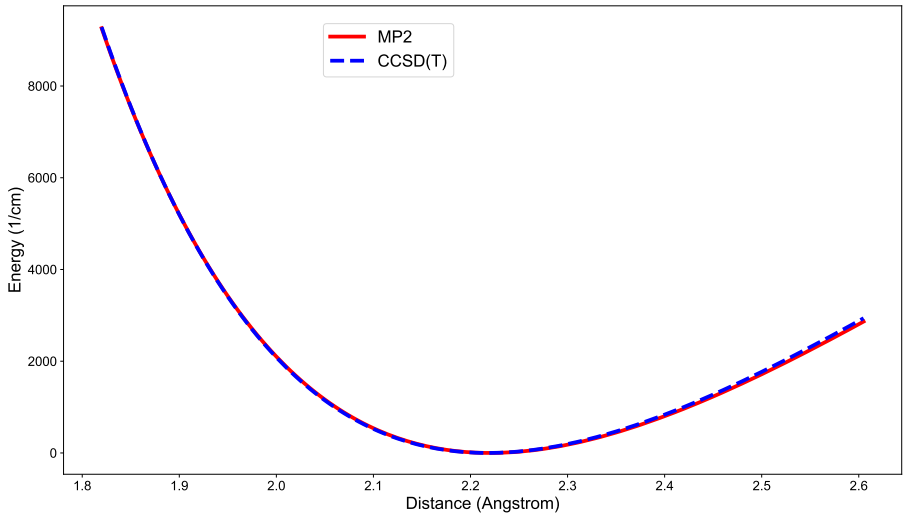

Fig. S37 Compound potassium fluoride (KF).

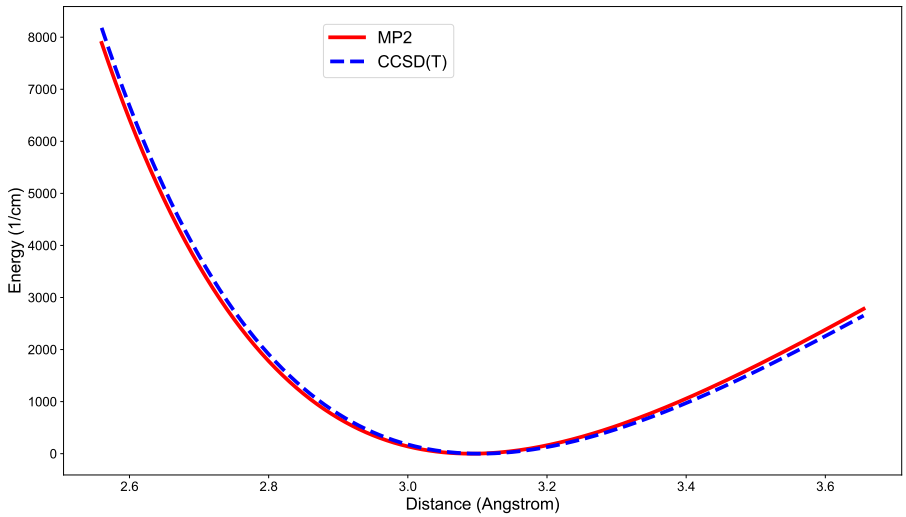

Fig. S38 Compound potassium iodide (KI).

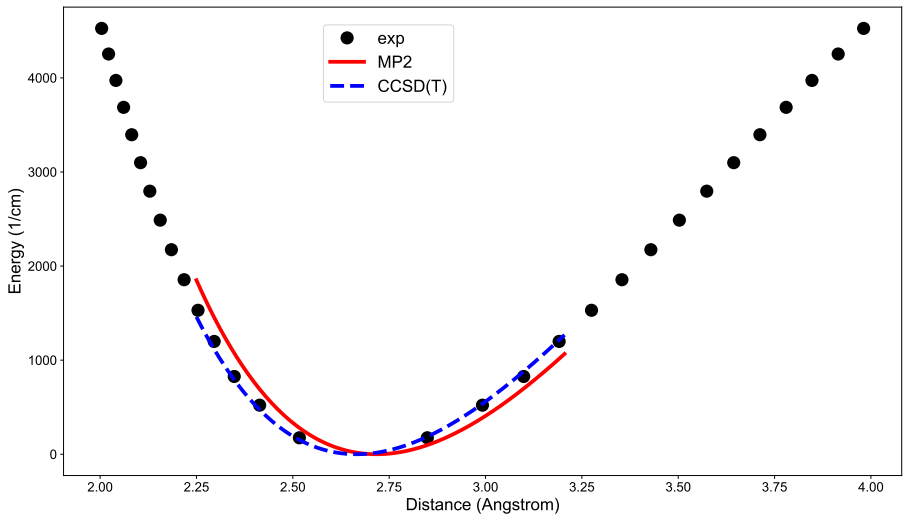

Fig. S39 Compound dilithium (Li_2). Experimental data from ref. 33.

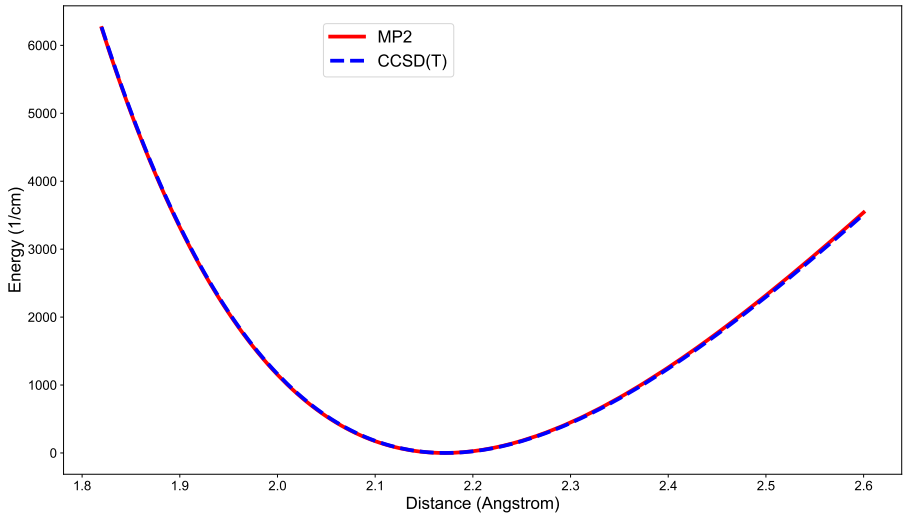

Fig. S40 Compound lithium bromide (LiBr).

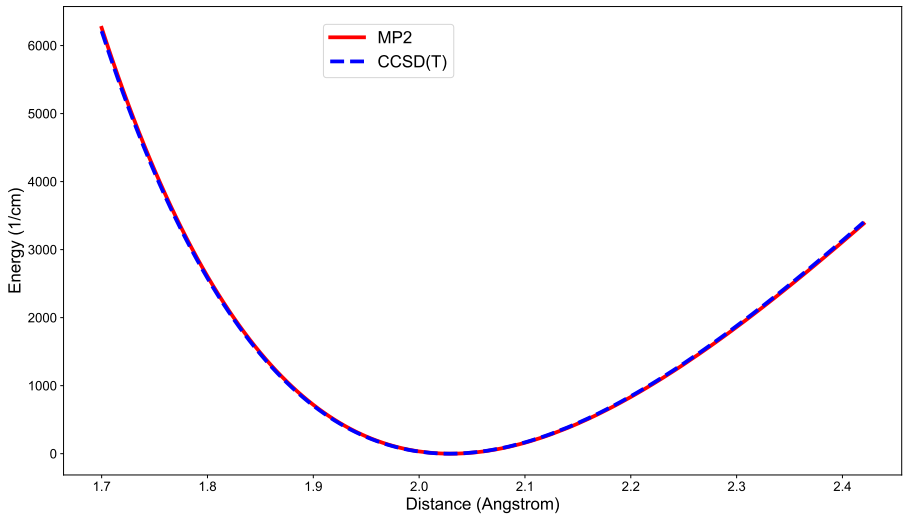

Fig. S41 Compound lithium chloride (LiCl).

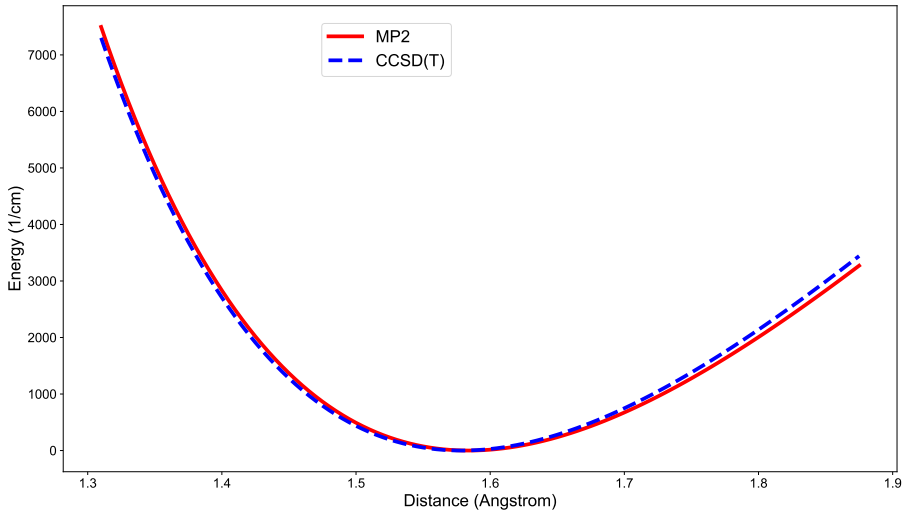

Fig. S42 Compound lithium fluoride (LiF).

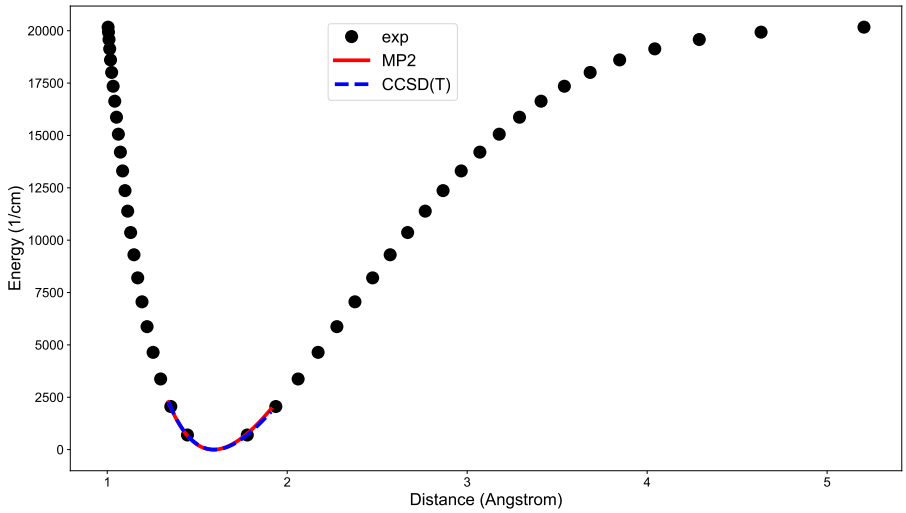

Fig. S43 Compound lithium hydride (LiH). Experimental data from ref. 34.

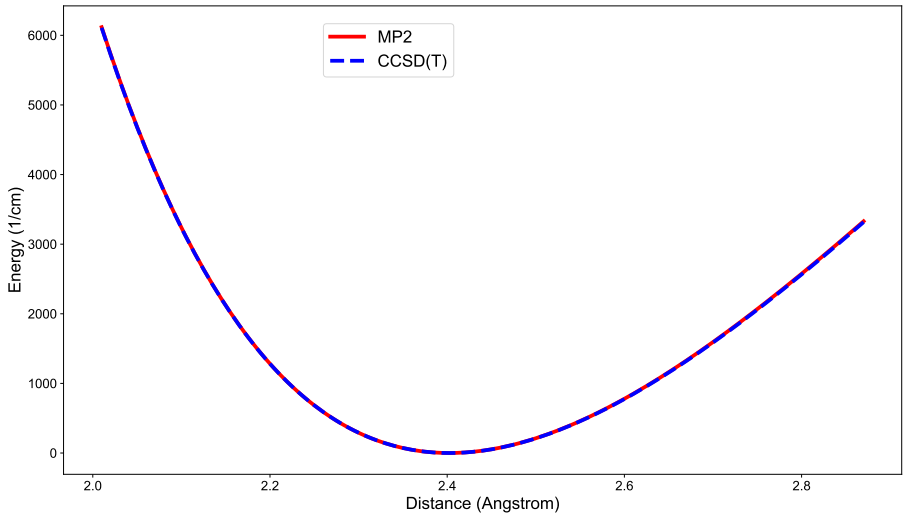

Fig. S44 Compound lithium iodide (LiI).

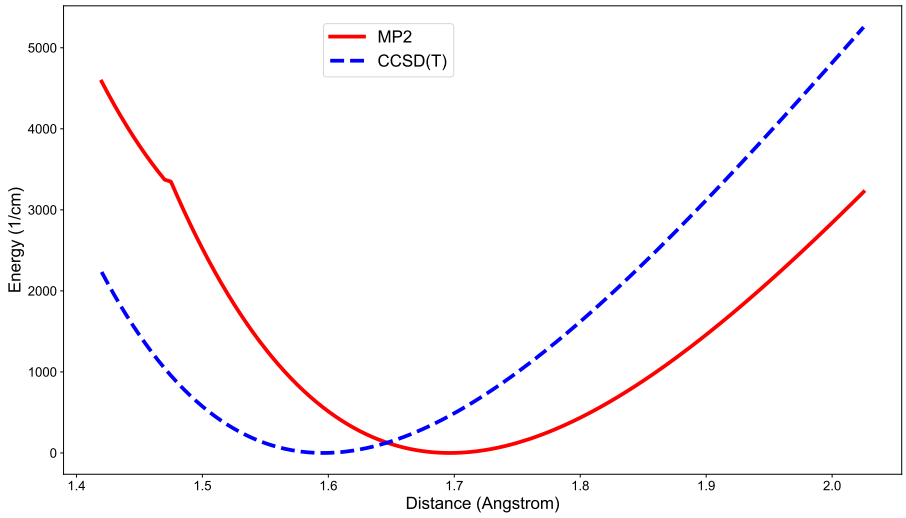

Fig. S45 Compound lithium monoxide (LiO).

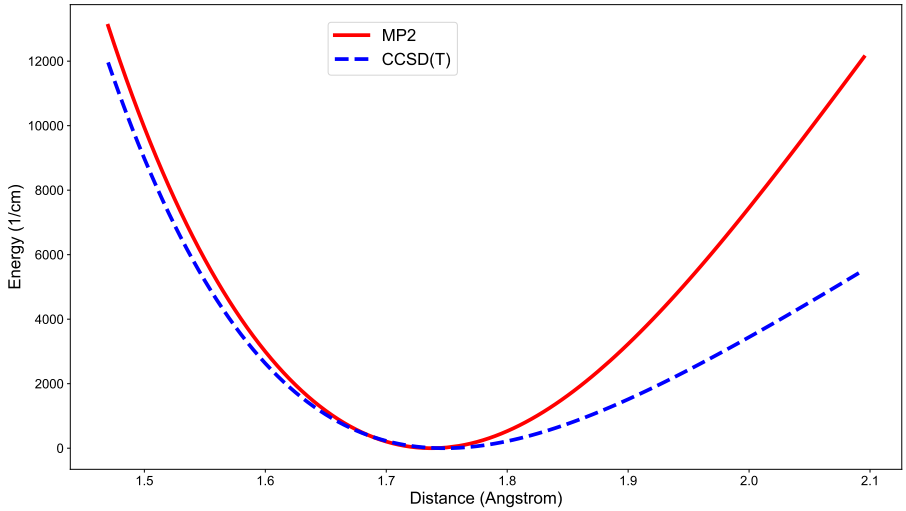

Fig. S46 Compound magnesium oxide (MgO).

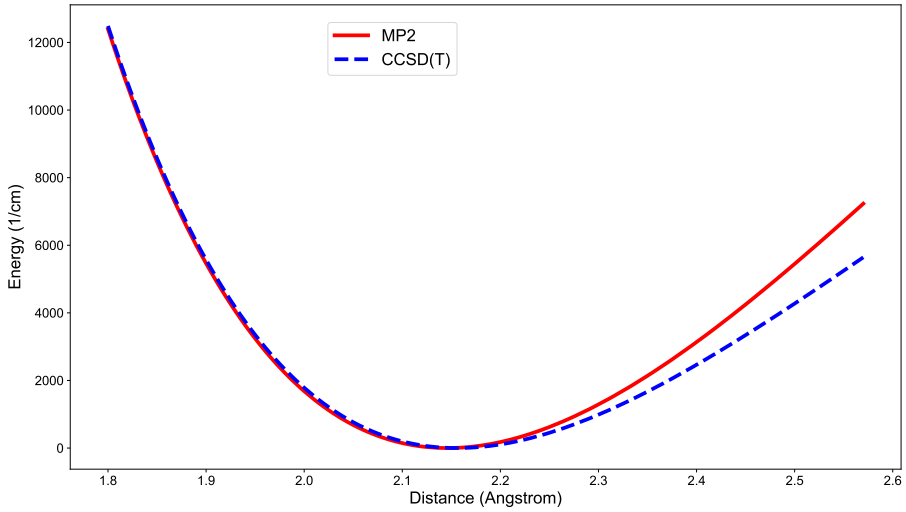

Fig. S47 Compound magnesium sulfide (MgS).

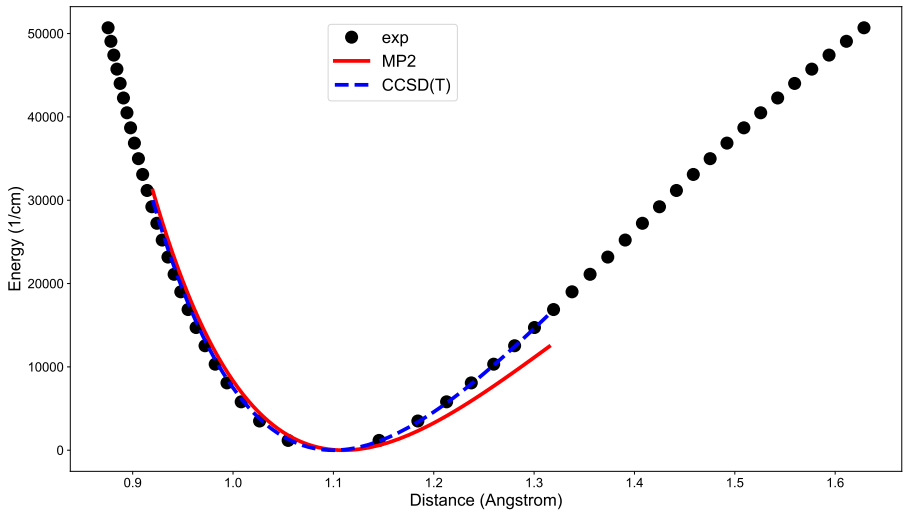

Fig. S48 Compound nitrogen (N_2). Experimental data from ref. 35.

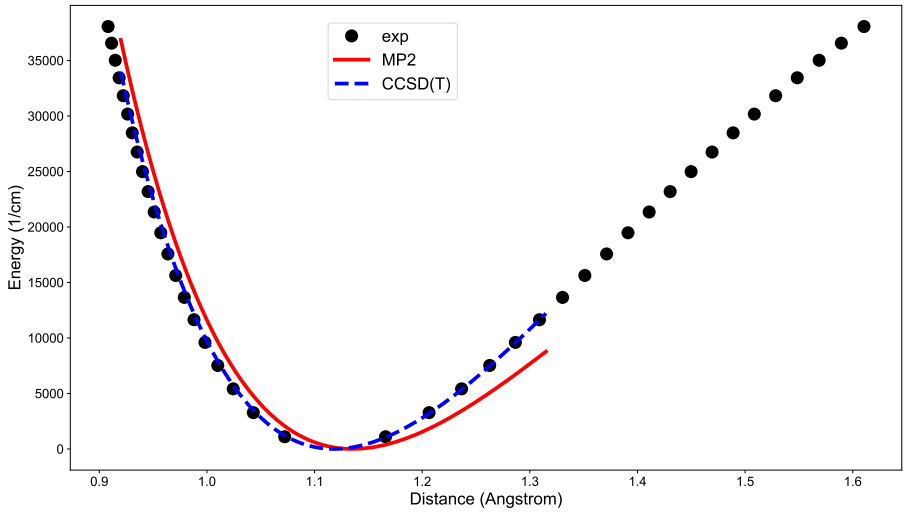

Fig. S49 Compound nitrogen ion (N_2^+). Experimental data from ref. 29.

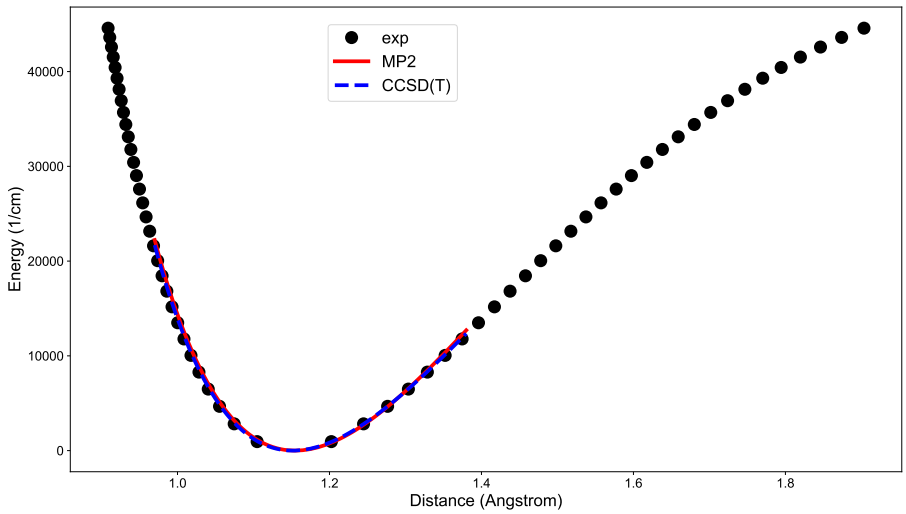

Fig. S50 Compound nitric oxide (NO). Experimental data from ref. 29.

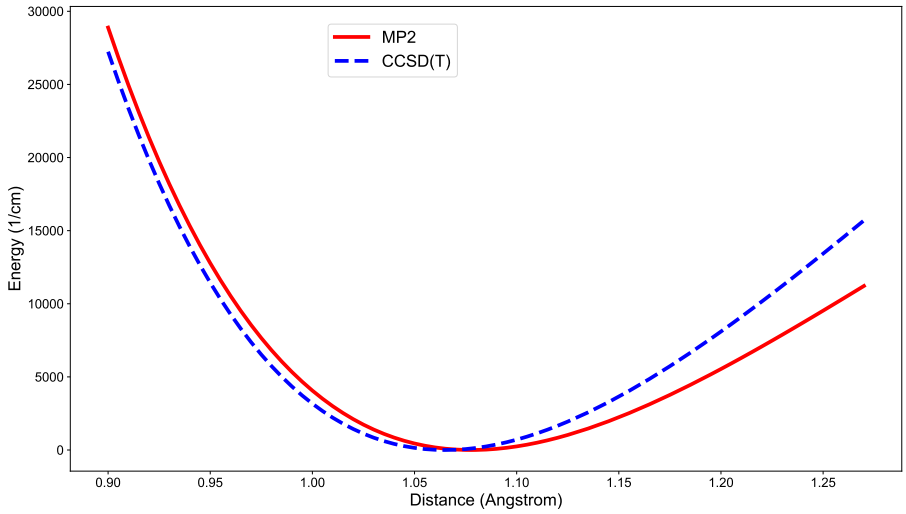

Fig. S51 Compound nitric oxide ion (NO^+).

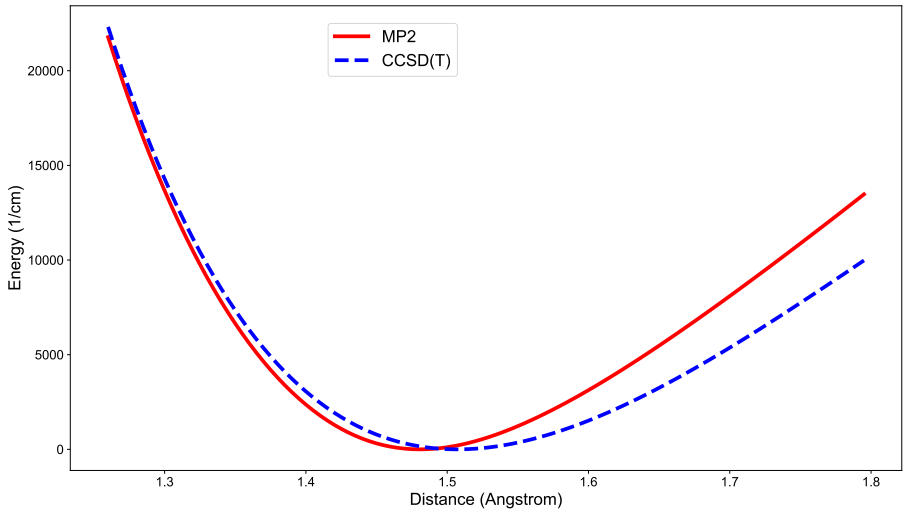

Fig. S52 Compound nitric sulfide (NS).

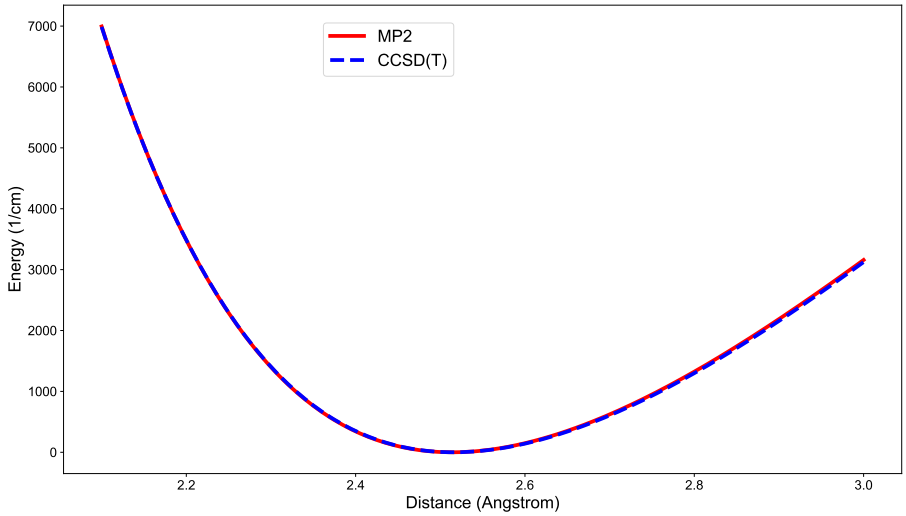

Fig. S53 Compound sodium bromide (NaBr).

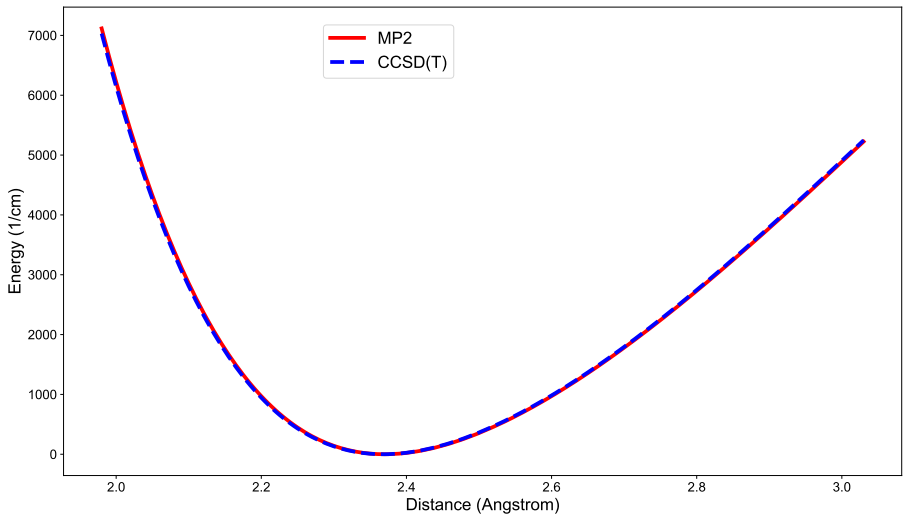

Fig. S54 Compound sodium chloride (NaCl).

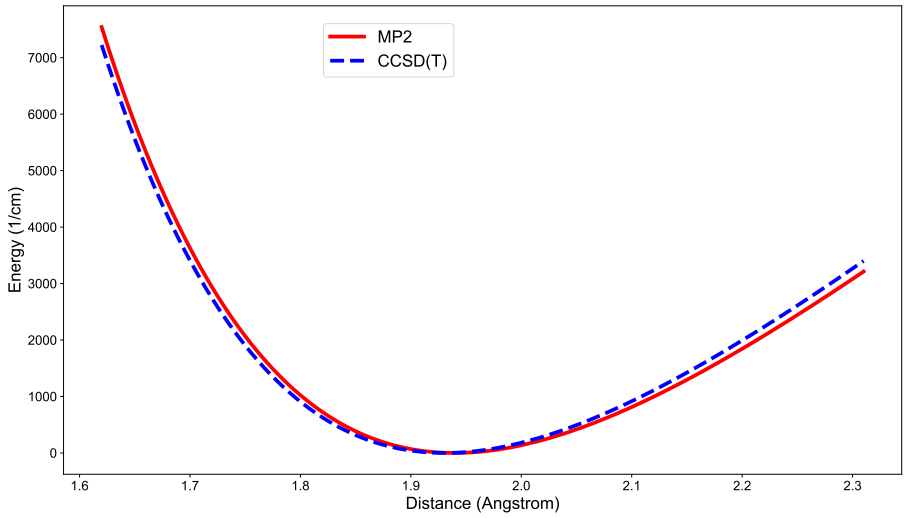

Fig. S55 Compound sodium fluoride (NaF).

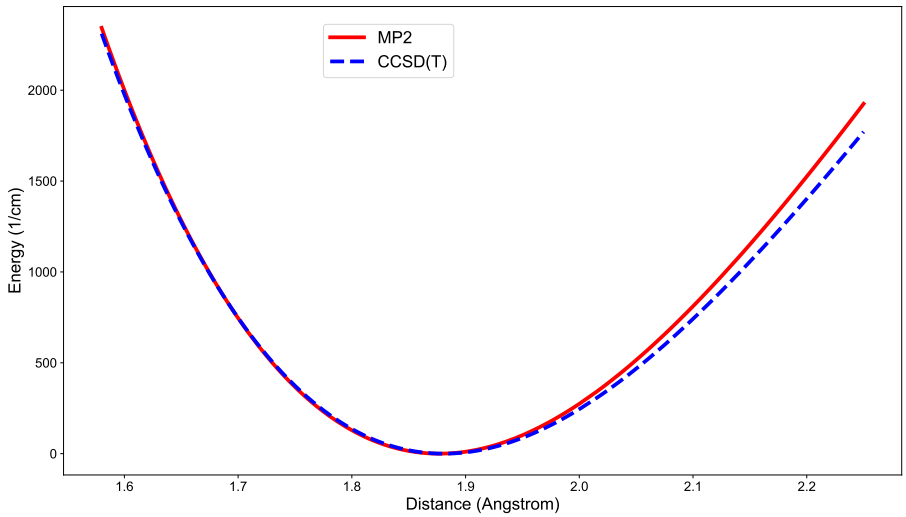

Fig. S56 Compound sodium hydride (NaH).

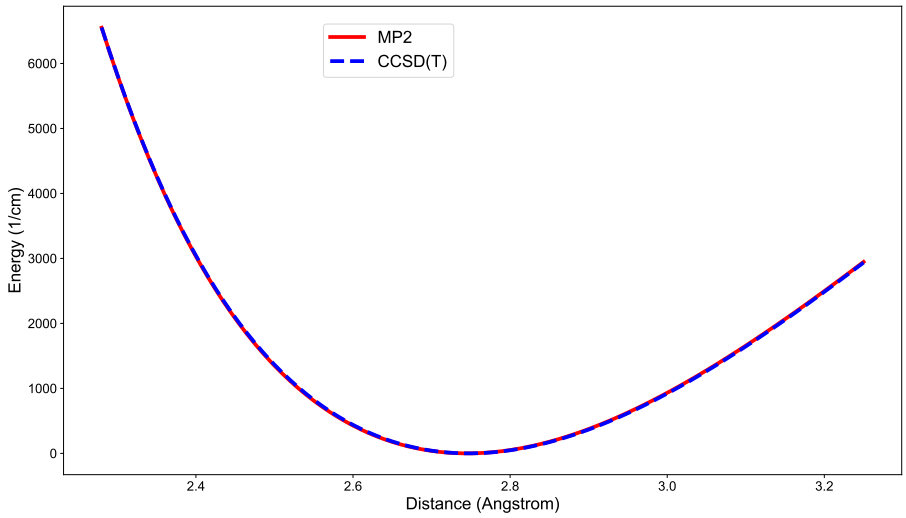

Fig. S57 Compound sodium iodide (NaI).

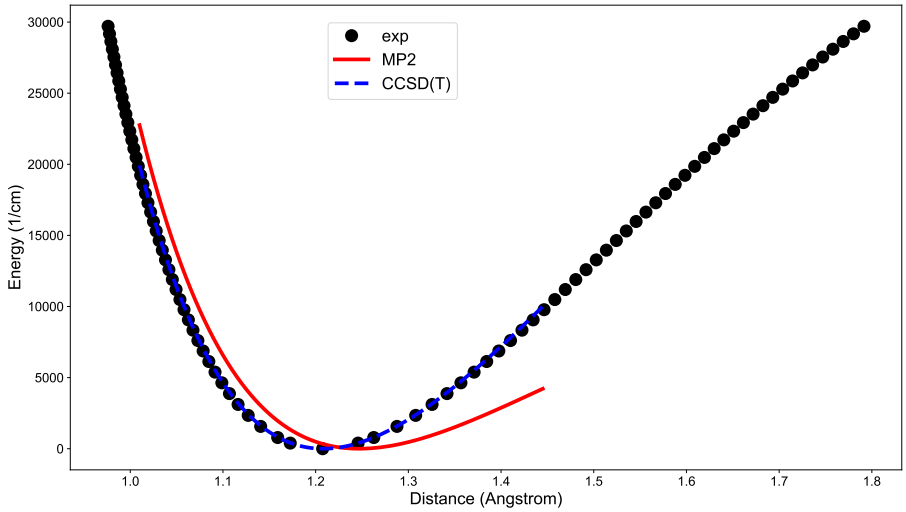

Fig. S58 Compound oxygen (O_2). Experimental data from ref. 36.

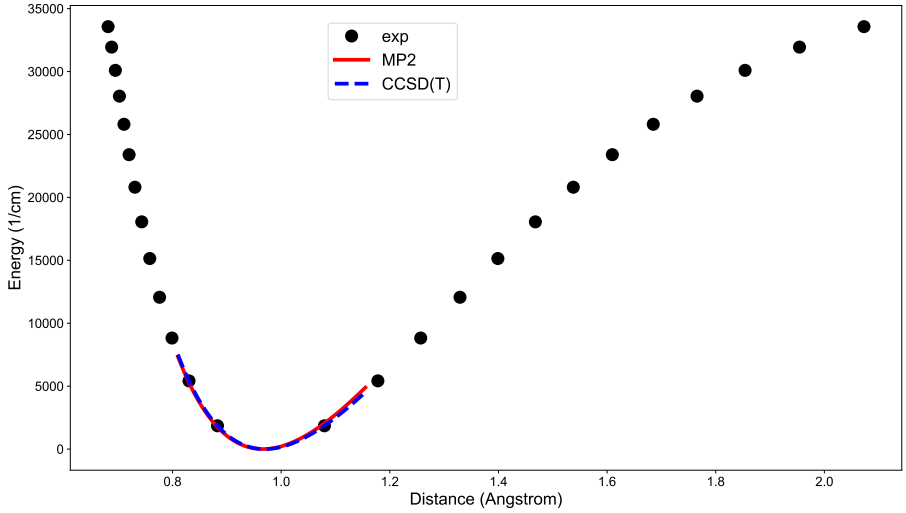

Fig. S59 Compound hydroxide (OH). Experimental data from ref. 29.

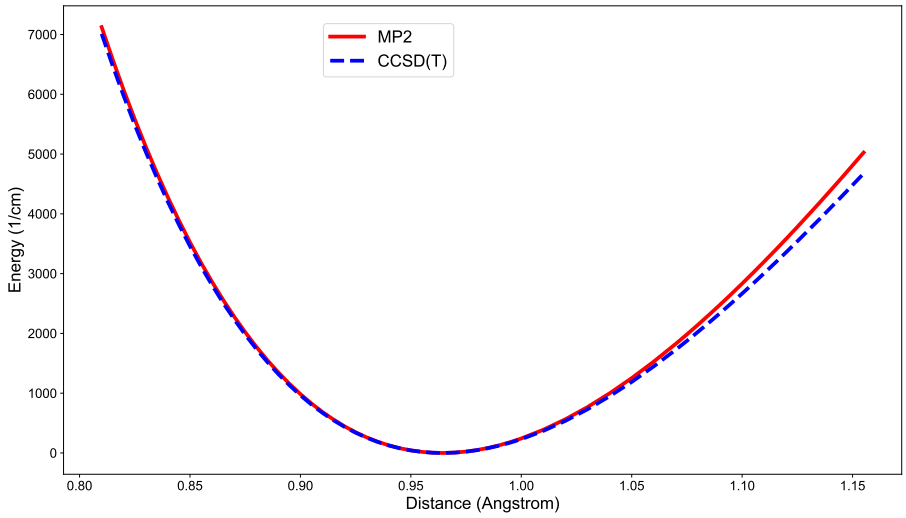

Fig. S60 Compound hydroxide (OH^-).

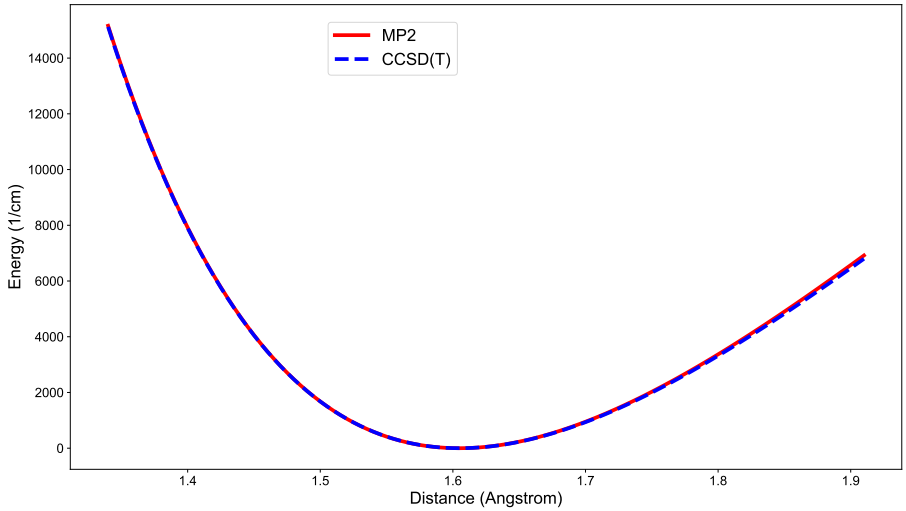

Fig. S61 Compound phosphorus monofluoride (PF).

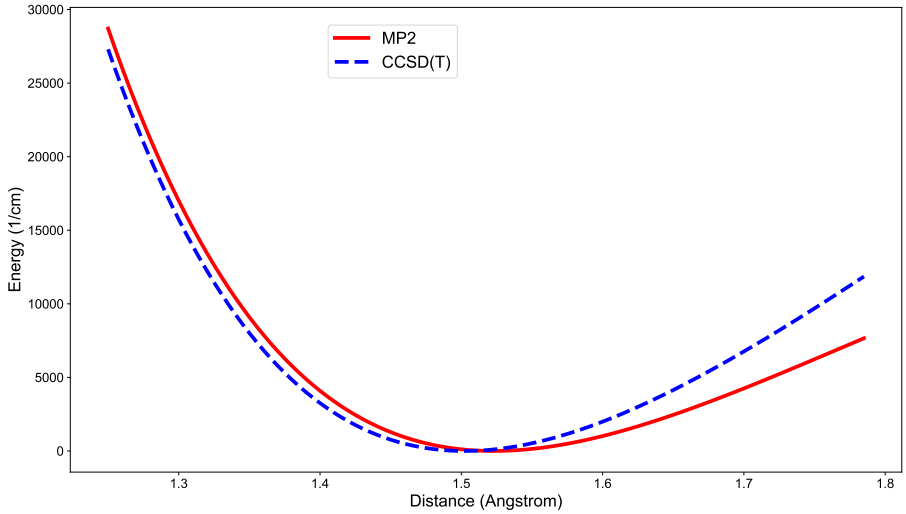

Fig. S62 Compound phosphor nitride (PN).

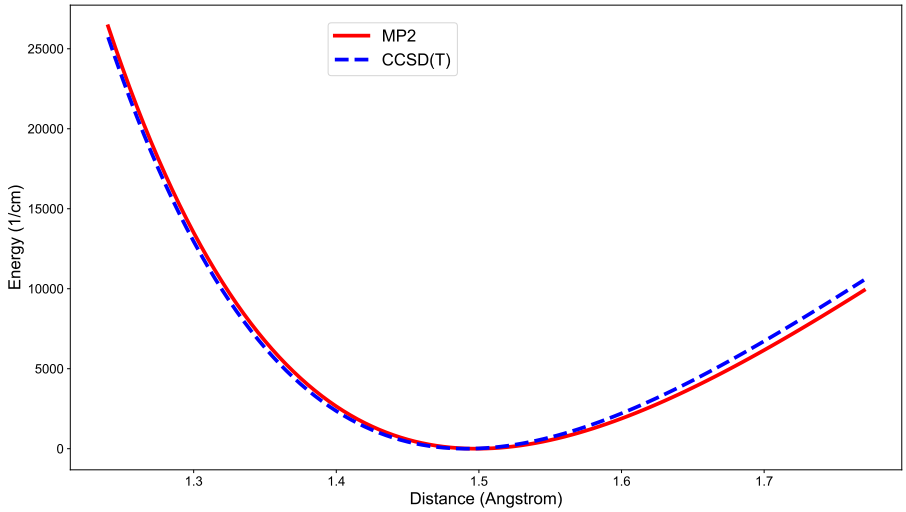

Fig. S63 Compound phosphorus monoxide (PO).

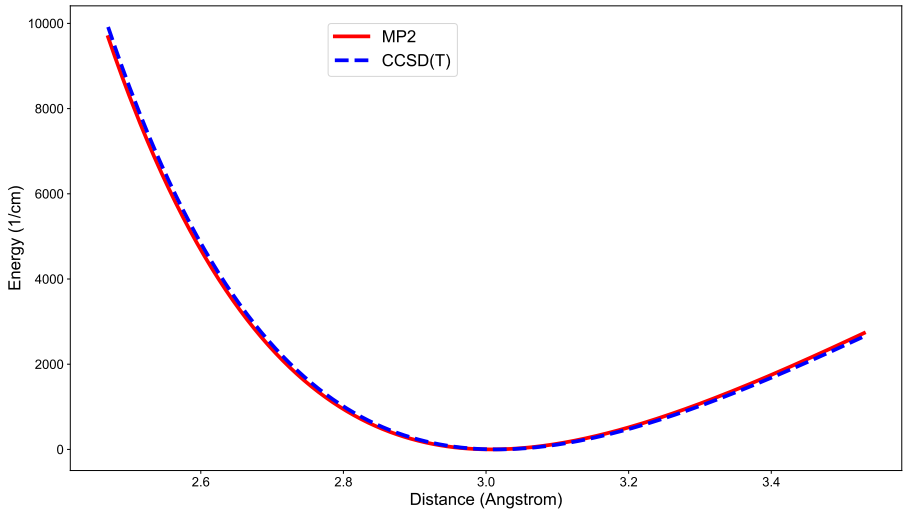

Fig. S64 Compound rubidium bromide (RbBr).

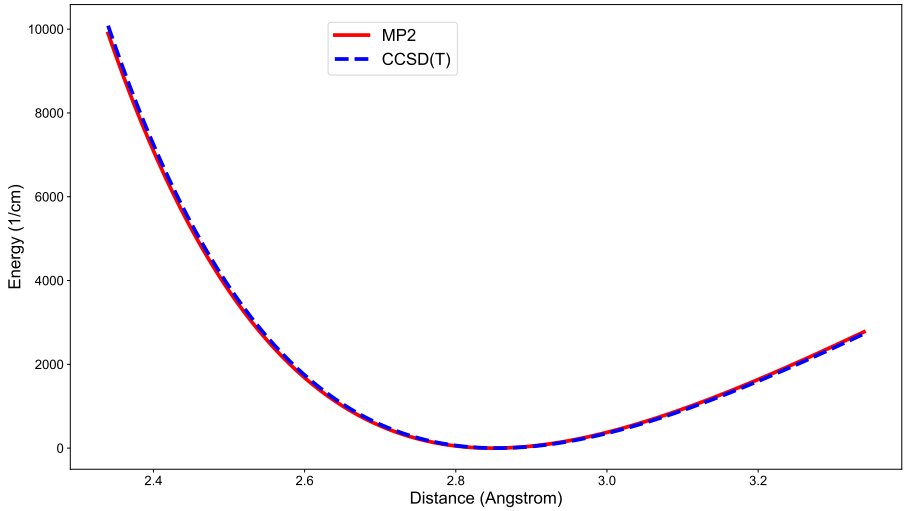

Fig. S65 Compound rubidium chloride (RbCl).

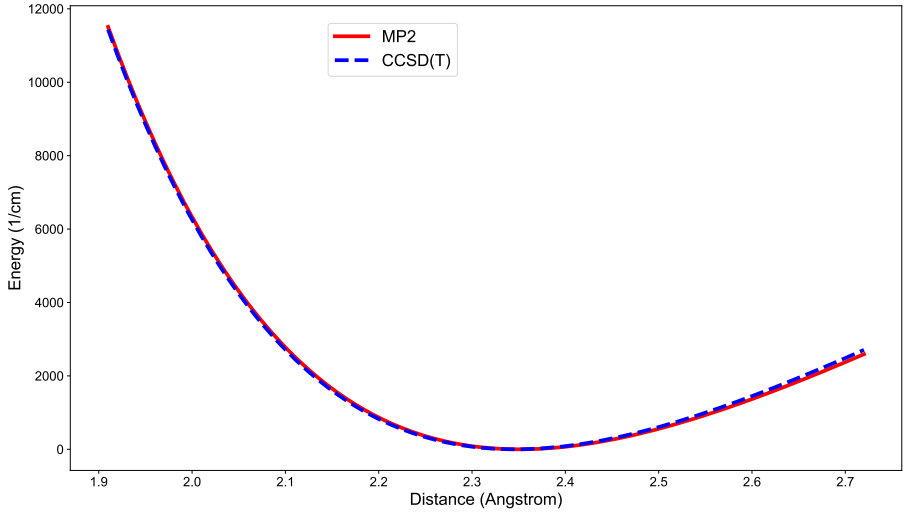

Fig. S66 Compound rubidium fluoride (RbF).

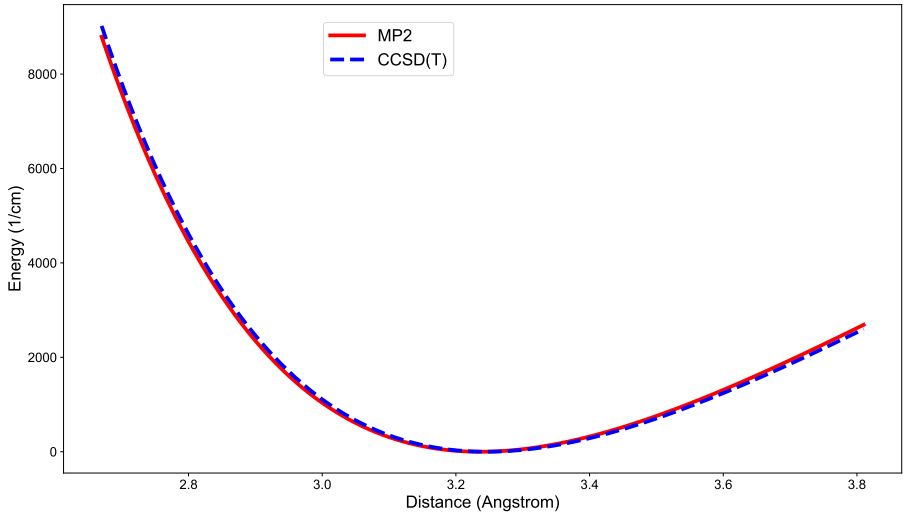

Fig. S67 Compound rubidium iodide (RbI).

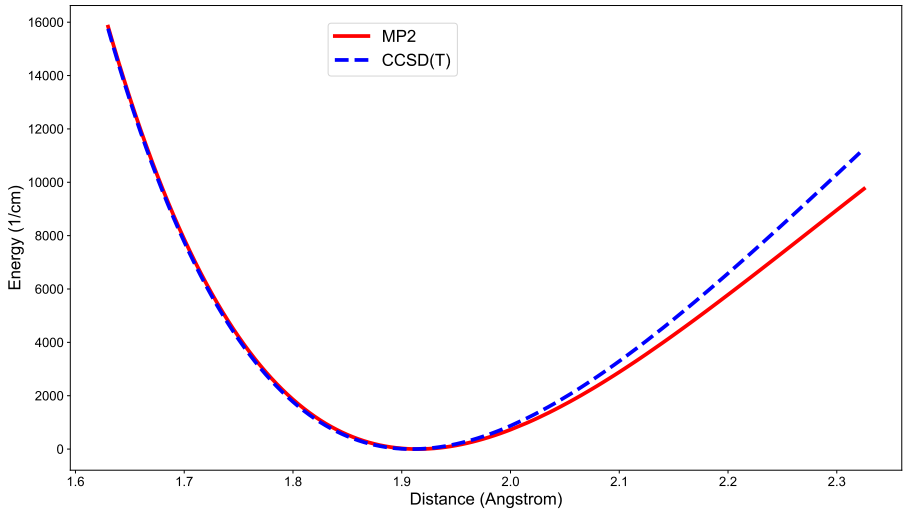

Fig. S68 Compound disulfur (S_2).

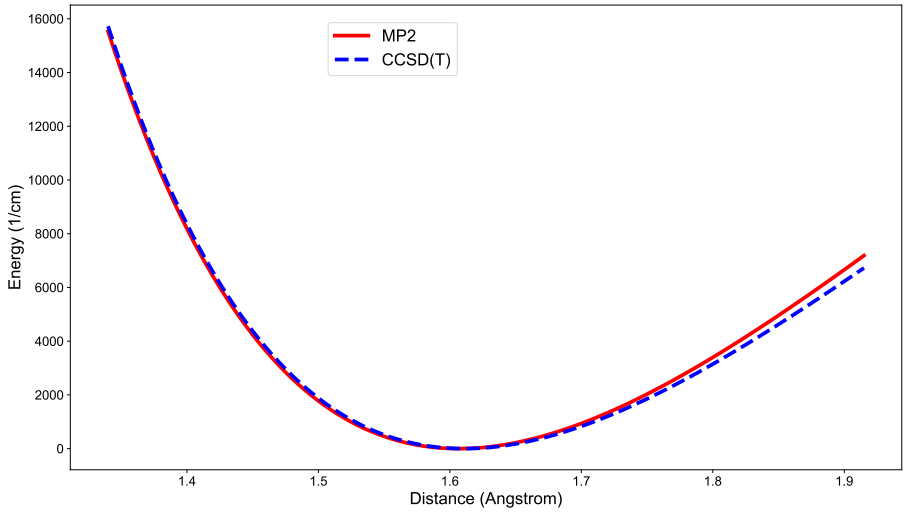

Fig. S69 Compound sulfur monofluoride (SF).

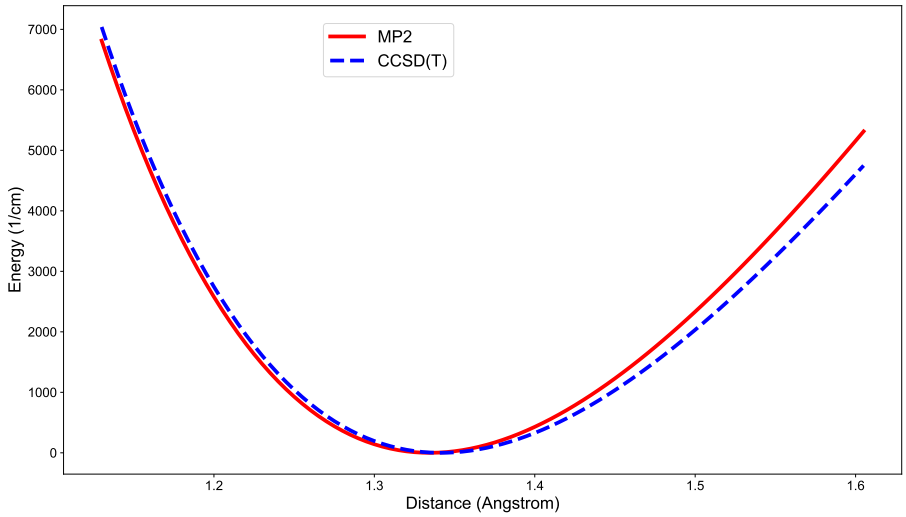

Fig. S70 Compound sulfur hydride (SH).

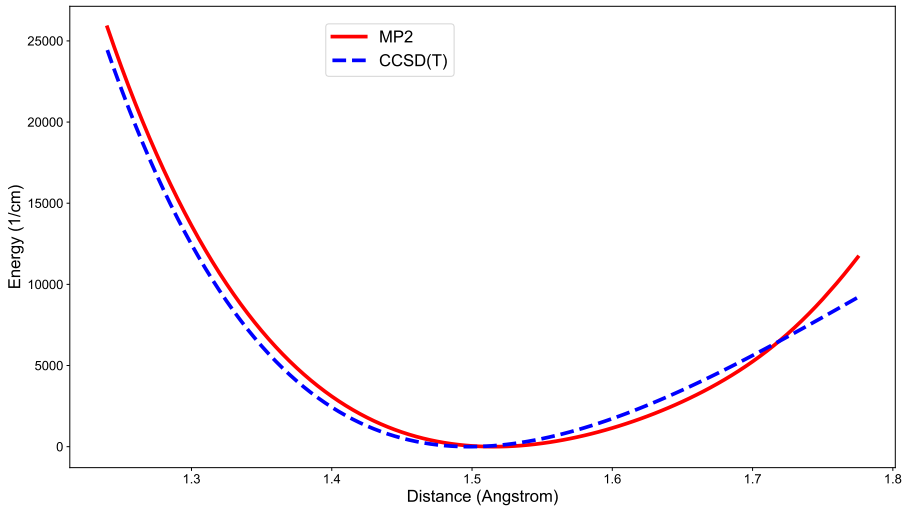

Fig. S71 Compound sulfur monoxide (SO).

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