Boiling, Critical and Freezing Temperatures in Light of Molecular Descriptors: Correlation and Causation

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Table S1*:

The available experimental normal boiling points (NBPs), critical temperatures (CTs) and normal freezing points (NFPs) in Kelvins of 169 compounds tabulated against molecular surface descriptors as defined in Methodology section.

Fluid	Group	NBP	CT	NFT	A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	S	g	g'
He	I	4.22	5.20		22.8	0	0.91	20.3	0	0	0	0	-
Ne	I	27.10	44.40	24.56	29.1	0	1.18	1.3	0	0	0	0	-
Ar	I	87.50	150.86	83.80	49.9	0	2.90	5.2	0	0	0	0	-
Kr	I	119.73	209.48	115.78	57.8	0	3.80	7.5	0	0	0	0	-
Xe	I	165.05	289.73	161.40	70.1	0	5.27	12.7	0	0	0	0	-
H_2	I	20.37	33.18	13.99	32.4	2,850	2.02	28.9	108	0.89	0	1	-
N_2	I	77.40	126.19	63.30	54.4	6,923	3.02	8.5	79	0.84	0	1	-
CO	I	81.63	134.45	68.05	55.0	41,752	3.14	13.1	419	2.69	0	1	-
F_2	I	85.20	144.00	55.20	47.0	4,290	2.14	2.5	111	0.78	0	1	-
O_2	I	90.20	154.58	54.80	50.3	0	2.60	3.8	5	0	1	1	-
NO	I	121.41	180.30	109.55	52.0	15,711	2.78	6.6	255	1.91	1	1	-
FCl	I	173.10		117.60	64.2	56,075	3.66	7.4	937	3.01	0	1	-
HCl	I	188.00	324.70	158.98	58.0	99,315	3.84	8.6	1,387	3.08	0	1	-
HBr	I	206.77	363.20	186.35	65.2	89,370	4.73	11.2	956	2.62	0	1	-
HI	I	237.60	424.00	222.39	77.0	83,420	6.20	17.1	607	2.14	0	1	-
Cl_2	I	239.50	416.96	171.65	80.6	38,474	5.26	9.8	390	1.35	0	1	-
ClBr	I	278.15		207.15	86.9	58,434	6.01	11.7	614	2.16	0	1	-
HF	I	292.70	461.00	190.00	36.5	180,771	1.83	2.8	5,012	6.39	0	1	-
Br_2	I	331.95	588.15	201.15	93.2	69,578	6.78	13.2	583	1.59	0	1	-
ClI	I	370.15		300.53	97.5	105,151	7.28	16.7	863	3.51	0	1	-
IBr	I	389.15		313.15	103.7	97,744	8.07	17.8	734	2.33	0	1	-
OF_2	I	127.90		49.40	61.4	18,500	2.88	3.7	235	1.54	0	2	-
O_3	I	161.30	261.15	80.70	64.4	58,205	3.40	4.9	587	3.28	0	2	-
N_2O	I	184.68	309.56	182.35	66.8	85,470	3.66	6.1	648	3.60	0	2	-
CO_2	I	194.69	304.18		64.6	169,433	3.40	4.6	1,391	3.76	0	1	-
SH_2	I	212.87	373.30	190.85	66.1	134,393	4.73	13.5	1,013	4.24	0	2	-
FNO	I	213.25			64.6	371,518	3.25	5.5	2,457	6.11	0	2	-
SOC	I	222.95	378.80	134.35	83.4	86,094	5.34	10.6	553	4.17	0	1	-
FCN	I	227.15		191.15	66.8	312,246	3.65	6.4	2,091	5.71	0	1	-
H_2Se	I	231.90	411.00	207.42	72.0	111,189	5.50	16.2	722	3.76	0	2	-
OCSe	I	251.45	394.25	148.75	88.7	90,120	6.00	12.6	636	3.60	0	1	-
SO_2	I	263.14	430.34	200.75	75.8	456,769	4.37	9.0	2,493	5.28	0	2	-
ClNO	I	267.35	440.65	210.65	83.6	401,496	5.01	9.4	1,598	3.91	0	2	-
Cl_2O	I	275.35		152.55	93.4	67,131	5.90	11.4	588	2.70	0	2	-
ClO_2	I	284.15	465.00	214.15	75.0	361,329	4.23	6.3	1,921	4.31	1	2	-
ClCN	I	286.15		266.60	83.6	439,475	5.22	9.5	2,383	5.37	0	1	-
NO_2	I	295.08	430.95	261.95	64.5	79,616	3.41	5.0	771	2.27	1	2	-
HCN	I	299.15	456.70	259.86	61.1	449,947	3.78	9.7	4,107	7.66	0	1	-
CS_2	I	319.35	552.00	161.45	101.3	24,706	7.44	15.3	147	0.79	0	1	-
BrCN	I	334.65		325.15	89.8	518,901	5.94	11.6	2,744	6.13	0	1	-
H2O	I	373.15	647.10	273.15	44.3	259,249	2.56	5.0	3,776	8.09	0	2	-

Fluid	Group	NBP	CT	NFT	A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	S	g	g'
CSe$_2$	I	398.65		229.55	111.3	44,880	8.89	18.3	249	0.93	0	1	-
NF$_3$	II	144.00	234.00	64.70	72.2	19,607	3.38	5.4	250	1.12	0	-	2
PF$_3$	II	171.35	271.20	121.65	84.5	244,452	4.39	12.0	1,426	3.12	0	-	2
BF$_3$	II	173.25	260.95	146.35	73.0	147,871	3.46	3.6	2,123	2.54	0	-	1
PH$_3$	II	185.40	324.50	139.35	73.3	48,356	5.35	21.3	473	2.65	0	-	2
F$_2$CO	II	188.65	287.85	161.95	73.5	140,014	3.56	4.3	1,661	6.13	0	-	1
FNO$_2$	II	200.80	349.45	107.20	75.5	88,531	3.77	4.6	907	3.54	0	-	1
AsH$_3$	II	210.65	373.05	157.15	77.8	27,816	5.89	23.8	304	2.54	0	-	2
NH$_3$	II	239.82	405.40	194.95	52.2	183,473	3.26	8.3	2,342	5.87	0	-	2
HFCO	II	246.65		130.95	68.0	405,976	3.57	7.0	2,846	6.50	0	-	1
NHF$_2$	II	250.00	403.00	157.15	65.8	274,387	3.27	6.6	2,845	4.09	0	-	2
CNCN	II	252.05	397.00	245.32	88.2	252,155	5.38	9.8	1,165	4.58	0	-	0
ClNO$_2$	II	257.25		128.15	91.9	117,007	5.30	8.5	687	2.95	0	-	1
ClO$_2$F	II	267.15		158.15	85.0	385,349	4.44	6.3	2,629	5.10	0	-	2
Cl$_2$CO	II	280.71	455.00	145.37	104.9	198,558	6.48	10.9	968	5.06	0	-	1
ClF$_3$	II	284.90	426.20	196.81	84.1	377,426	4.18	5.4	2,043	4.99	0	-	1
BCl$_3$	II	285.75	455.15	166.15	120.5	57,147	7.89	13.8	404	1.48	0	-	1
SO$_3$	II	317.65	491.00	289.95	84.6	279,896	4.52	5.5	2,442	3.14	0	-	1
BrO$_2$F	II	328.15		264.15	91.2	737,639	4.96	7.3	3,901	4.74	0	-	2
H$_2$CO	II	329.23	508.00	178.25	62.8	456,331	3.69	9.9	2,861	5.95	0	-	1
AsF$_3$	II	330.28		267.25	89.1	754,821	4.75	12.1	3,234	4.96	0	-	2
NCl$_3$	II	344.15		233.15	116.7	92,088	7.66	13.6	467	1.90	0	-	2
PCl$_3$	II	349.15	563.00	180.15	129.4	120,693	8.72	17.4	402	1.80	0	-	2
BBr$_3$	II	364.45	573.15	227.15	137.4	87,510	9.97	18.2	351	1.59	0	-	1
BrF$_3$	II	398.95		281.92	89.5	605,150	4.64	7.0	3,274	6.76	0	-	1
AsCl$_3$	II	403.15	654.00	257.15	134.7	327,976	9.19	18.0	960	2.78	0	-	2
PBr$_3$	II	446.35	711.00	231.65	146.4	163,856	10.84	20.7	368	1.71	0	-	2
BI$_3$	II	482.65		322.85	166.0	146,591	13.62	29.6	298	1.61	0	-	1
AsBr$_3$	II	494.15		304.25	151.4	330,190	11.32	21.4	725	2.44	0	-	2
CH$_4$	III	111.00	190.60	90.60	59.7	4,966	3.73	14.3	62	0.57	0	-	-
CF4	III	145.10	227.50	89.57	81.3	18,165	3.69	3.8	316	0.61	0	-	-
SiH$_4$	III	161.15	269.69	88.15	80.5	2,926	5.63	30.4	141	0.17	0	-	-
SiH$_3$F	III	174.55			83.2	222,574	5.13	25.8	1,907	5.12	0	-	-
SiHF$_3$	III	178.15		141.75	89.0	360,464	4.56	12.6	1,931	3.85	0	-	-
GeH$_4$	III	183.15	312.20	108.15	83.0	827	5.97	31.3	98	0.10	0	-	-
SiF$_4$	III	187.00	259.00	182.95	92.7	176,656	4.41	4.3	1,487	2.24	0	-	-
CHF$_3$	III	191.09	299.01	117.97	75.9	238,080	3.63	6.2	1,628	2.98	0	-	-
CF$_3$Cl	III	191.74	302.00	92.15	96.5	48,005	5.01	7.6	304	1.21	0	-	-
CH$_3$F	III	195.00	317.40	129.85	65.1	268,472	3.60	11.7	1,749	4.25	0	-	-
SiH$_2$F$_2$	III	195.30		151.15	85.9	395,067	4.79	19.9	2,046	4.78	0	-	-
CF$_3$Br	III	215.26	340.15	105.15	102.6	59,841	5.62	9.6	382	1.32	0	-	-
SnH$_4$	III	221.15		127.15	93.2	29,833	7.05	38.9	316	0.63	0	-	-
CH$_2$F$_2$	III	221.50	351.26	136.35	70.5	386,448	3.59	9.1	1,893	4.61	0	-	-
CHF$_2$Cl	III	232.32	369.30	115.73	91.8	227,101	5.05	9.7	1,216	3.62	0	-	-
SF$_4$	III	236.00	364.10	152.00	91.3	281,449	4.43	6.4	1,559	5.06	0	-	-
GeF$_4$	III	236.70			99.5	321,837	4.85	4.4	2,338	2.66	0	-	-
SiF$_2$Cl$_2$	III	241.00	369.00	229.15	123.5	156,731	7.15	11.1	820	3.10	0	-	-
SiH$_3$Cl	III	242.75		155.15	99.6	203,376	6.77	26.3	993	2.85	0	-	-
CF$_2$Cl$_2$	III	243.42	384.95	115.16	110.7	61,260	6.35	10.7	302	2.23	0	-	-

Fluid	Group	NBP	CT	NFT	A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	S	g	g'
CH_3Cl	III	247.00	416.00	175.55	81.7	281,523	5.24	14.4	1,015	3.40	0	-	-
CF_3I	III	251.34	395.00		113.3	101,810	6.68	14.7	543	1.76	0	-	-
CHF_2Br	III	257.67	411.98	128.00	98.1	241,008	5.70	11.6	1,171	3.52	0	-	-
CH_2FCl	III	264.00	427.00	138.05	86.9	342,702	5.11	12.0	1,484	4.84	0	-	-
CF_2ClBr	III	269.14	426.15	113.65	116.6	74,965	6.99	12.5	383	2.30	0	-	-
CH_3Br	III	276.60	467.00	179.55	88.1	284,354	5.99	16.0	933	3.44	0	-	-
SiH_2Cl_2	III	281.30	449.15	151.15	117.9	220,235	7.88	22.4	834	2.30	0	-	-
$CHFCl_2$	III	282.01	451.60	138.15	106.6	212,484	6.48	12.5	999	3.49	0	-	-
$SiFCl_3$	III	285.40	438.41		137.8	84,372	8.54	13.9	441	3.67	0	-	-
CH_2FBr	III	292.15			93.2	352,905	5.81	13.8	1,398	4.67	0	-	-
CHF_2I	III	295.15		151.15	108.8	272,581	6.83	16.7	1,107	3.72	0	-	-
CF_2Br_2	III	295.94	471.30	163.05	122.5	90,031	7.64	14.2	405	2.31	0	-	-
$CFCl_3$	III	296.90	471.10	162.72	123.8	78,012	7.66	13.1	314	2.12	0	-	-
$SiHCl_3$	III	306.00	479.00	144.95	135.2	126,055	8.93	19.0	477	1.51	0	-	-
$CHFClBr$	III	309.26		158.15	112.6	227,527	7.16	14.2	974	3.40	0	-	-
CH_2Cl_2	III	312.90	510.00	178.01	102.2	297,232	6.65	14.6	1,053	3.40	0	-	-
CH_3I	III	315.70	527.95	207.00	98.8	291,472	7.27	20.6	814	3.22	0	-	-
CH_2FI	III	326.00			104.0	373,703	7.00	18.6	1,271	4.55	0	-	-
$SiCl_4$	III	330.80	508.10	204.41	151.3	37,022	9.91	16.3	193	0.58	0	-	-
$CHCl_3$	III	334.33	536.40	209.68	120.2	195,743	7.89	14.8	752	2.41	0	-	-
$CHFBr_2$	III	338.00		195.15	118.5	244,057	7.85	15.9	953	3.32	0	-	-
CH_2ClBr	III	341.20	557.00	185.20	108.3	302,798	7.37	16.2	989	3.21	0	-	-
CCl_4	III	349.79	556.35	250.33	135.7	96,091	8.91	15.0	268	1.13	0	-	-
$CFClBr_2$	III	353.00			135.0	113,691	8.97	16.3	419	2.15	0	-	-
$GeCl_4$	III	359.70	553.20	221.65	157.3	58,238	10.39	17.2	290	0.70	0	-	-
$CHCl_2Br$	III	363.20		216.00	126.0	209,682	8.57	16.4	737	2.30	0	-	-
CH_2Br_2	III	370.15	610.00	221.05	114.2	309,286	8.11	17.8	926	3.03	0	-	-
CF_2I_2	III	374.15		201.15	142.8	157,790	9.94	23.3	540	2.73	0	-	-
$CHFBrI$	III	376.00			128.7	274,741	9.03	20.5	927	3.37	0	-	-
$CHFI_2$	III	373.45		238.65	138.8	306,757	10.23	24.8	898	3.35	0	-	-
CCl_3Br	III	376.65		267.55	141.1	114,585	9.56	16.4	349	1.18	0	-	-
$CFBr_3$	III	379.50		199.15	140.5	135,052	9.63	17.7	438	2.13	0	-	-
CH_2ClI	III	382.00			118.6	320,557	8.59	20.8	904	2.91	0	-	-
$SnCl_4$	III	387.30	591.90	239.08	168.6	110,895	11.29	18.2	598	0.82	0	-	-
$CHClBr_2$	III	393.00		253.15	131.6	225,740	9.26	17.9	725	2.23	0	-	-
$CHCl_2I$	III	404.00			135.9	236,083	9.74	20.8	724	2.21	0	-	-
CH_2BrI	III	409.15		274.00	124.5	328,156	9.35	22.2	855	2.78	0	-	-
$CHBr_3$	III	422.35	696.00	281.20	137.2	243,776	9.96	19.3	711	2.18	0	-	-
CCl_2Br_2	III	423.35		311.15	146.4	135,735	10.21	17.8	366	1.23	0	-	-
$SiBr_4$	III	427.00	663.00	278.54	172.4	94,003	12.51	21.5	194	0.85	0	-	-
CH_2I_2	III	455.15		279.15	134.6	347,829	10.62	26.5	784	2.56	0	-	-
$GeBr_4$	III	459.50	718.00	299.25	178.3	119,420	13.04	22.6	263	0.98	0	-	-
$CHClI_2$	III	473.00		269.15	151.1	283,703	11.63	26.1	694	2.03	0	-	-
$SnBr_4$	III	478.00	744.00	304.00	189.8	142,904	14.00	24.0	436	0.93	0	-	-
CCl_3I	III			265.35	150.5	145,471	10.67	20.5	465	1.37	0	-	-
CH_3SH	III	279.11	469.95	150.18	88.6	241,847	6.01	18.2	1,016	3.64	0	-	-
CH_3OH	III	337.85	512.64	175.47	70.9	263,663	4.24	12.6	2,514	7.16	0	-	-
CH_3NH_2	III	266.82	430.05	179.69	77.1	173,901	4.84	14.8	1,684	5.38	0	-	-
CH_3CH_3	IV	184.55	305.32	90.35	83.5	7,199	5.26	19.3	49	0.67	0	-	-

Fluid	Group	NBP	CT	NFT	A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	S	g	g'
CH_3CH_2F	IV	235.45	375.31	129.95	88.4	334,482	5.13	16.6	1,512	4.14	0	-	-
CH_2FCH_2F	IV	283.65			93.7	485,876	5.06	14.0	1,337	3.86	0	-	-
CH_3CH_2Cl	IV	285.42	460.35	136.75	103.4	368,419	6.65	18.8	923	3.40	0	-	-
CH_3CH_2Br	IV	311.50	503.80	154.55	109.4	384,793	7.36	20.1	873	3.46	0	-	-
CH_3CH_2I	IV	345.45	561.00	162.05	119.6	399,077	8.55	24.2	781	3.25	0	-	-
CH_2ClCH_2Cl	IV	356.59	561.60	237.49	123.2	384,522	7.99	18.3	758	2.84	0	-	-
CH_2BrCH_2Br	IV	404.51	650.15	282.94	135.2	393,794	9.42	20.9	705	2.62	0	-	-
CH_2ICH_2I	IV	473.16		356.16	155.6	436,934	11.88	29.1	644	2.33	0	-	-
Cyclopropane	IV	240.00	398.00	146.00	93.0	59,448	5.88	17.4	251	2.26	0	-	-
CH_3CH_2SH	IV	308.15	499.15	125.26	109.5	289,644	7.35	21.8	953	3.61	0	-	-
CH_3CH_2OH	IV	351.44	513.92	159.05	93.4	316,314	5.71	17.3	2,297	6.65	0	-	-
$CH_3CH_2NH_2$	IV	289.73	456.15	192.15	98.9	187,254	6.29	18.9	1,214	5.18	0	-	-
CH_2SHCH_2SH	IV	419.20		231.95	135.4	580,583	9.43	24.2	1,057	4.08	0	-	-
CH_2OHCH_2OH	IV	470.45	720.00	260.15	103.4	756,363	6.17	15.3	2,825	7.96	0	-	-
$CH_3CH_2CH_3$	IV	231.11	369.83	85.47	104.8	12,631	6.67	22.8	54	0.76	0	-	-
CH_3CHFCH_3	IV	263.81		139.80	108.9	374,044	6.50	20.0	1,341	3.94	0	-	-
$CH_3CH_2CH_2F$	IV	269.95		114.16	109.7	405,073	6.51	20.2	1,390	3.60	0	-	-
$CH_3CHClCH_3$	IV	308.85		155.97	122.2	424,692	7.89	21.6	857	3.39	0	-	-
$CH_3CH_2CH_2Cl$	IV	319.67	503.15	150.35	124.6	454,316	8.02	22.3	887	3.20	0	-	-
$CH_3CHBrCH_3$	IV	333.00	532.00	184.20	127.8	457,232	8.55	22.7	824	3.31	0	-	-
$CH_3CH_2CH_2Br$	IV	344.15	536.94	163.15	130.6	476,137	8.72	23.6	841	3.25	0	-	-
CH_3CHICH_3	IV	362.40		183.15	137.4	481,442	9.67	26.2	752	3.22	0	-	-
$CH_3CH_2CH_2I$	IV	375.60		171.85	140.8	492,594	9.90	27.7	757	3.10	0	-	-
$CH_3CHSHCH_3$	IV	328.00	517.30	142.61	127.5	311,935	8.52	23.8	879	3.65	0	-	-
$CH_3CH_2CH_2SH$	IV	339.80	533.00	167.23	130.6	344,246	8.72	25.2	919	3.48	0	-	-
$CH_3CHOHCH_3$	IV	355.50	509.00	185.75	113.1	338,159	7.02	20.4	2,122	6.26	0	-	-
$CH_3CH_2CH_2OH$	IV	370.35	536.78	146.95	114.6	365,465	7.09	20.8	2,180	6.25	0	-	-
$CH_2NH_2CH_2NH_2$	IV	390.41	613.10	284.29	114.1	522,945	7.31	18.5	1,714	5.82	0	-	-
$CH_3CHNH_2CH_3$	IV	304.92	471.90	177.95	117.8	226,757	7.54	21.5	1,187	4.98	0	-	-
$CH_3CH_2CH_2NH_2$	IV	321.00	496.95	190.15	120.0	255,086	7.64	22.5	1,380	4.75	0	-	-

[*] The available experimental normal boiling points (NBPs), critical temperatures (CTs) and normal freezing points (NFPs), in Kelvins, of the studied fluids were laboriously and scrupulously compiled, filtered and mainly doubled-checked, from different reputable sources and peer-reviewed literature.[1-18] Some fluids properties were extracted from or double checked in dedicated works.[19-34] Safety datasheets of some laboratories and reputable institutions were also made use of to augment our datasets accuracy as much as possible.[35-40]

Table S2:

The dependence table of normal boiling points (NBPs) of 42 mono-, di- and triatomic compounds. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group I (42 NBP's) Variables	R	Adj. R^2	SE	A coeff / p-val	Γ_s coeff / p-val	P_{av} coeff / p-val	L_{av} coeff / p-val	Γ_m coeff / p-val	$\sigma_{r,ep}$ coeff / p-val	S coeff / p-val	g coeff / p-val	Intercept
A	0.764	0.573	67.32	3.84 / 4.08×10^{-9}								-47.42
$A + \Gamma_s$	0.830	0.673	58.84	3.48 / 3.59×10^{-9}	2.27×10^{-4} / 7.57×10^{-4}							-52.42
$A + \Gamma_s + P_{av}$	0.851	0.702	56.20	0.04 / 9.81×10^{-1}	2.80×10^{-4} / 9.28×10^{-5}	38.99 / 3.55×10^{-2}						6.28
$A + \Gamma_s + P_{av} + L_{av}$	0.876	0.742	52.34	-2.76 / 1.47×10^{-1}	2.90×10^{-4} / 2.31×10^{-5}	76.45 / 1.32×10^{-3}	-5.38 / 1.31×10^{-2}					87.86
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m$	0.954	0.897	33.09	1.98 / 1.48×10^{-1}	-1.60×10^{-4} / 2.99×10^{-2}	27.85 / 7.76×10^{-2}	-1.25 / 3.84×10^{-1}	6.31×10^{-2} / 6.85×10^{-9}				-74.10
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.954	0.894	33.52	1.85 / 2.04×10^{-1}	-1.63×10^{-4} / 3.10×10^{-2}	29.12 / 8.08×10^{-2}	-1.33 / 3.71×10^{-1}	6.05×10^{-2} / 3.19×10^{-5}	1.77 / 7.84×10^{-1}			-72.16
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + S$	0.964	0.914	30.16	1.43 / 2.76×10^{-1}	-1.78×10^{-4} / 1.02×10^{-2}	34.56 / 2.45×10^{-2}	-.86 / 5.19×10^{-1}	6.03×10^{-2} / 7.18×10^{-6}	4.12 / 4.83×10^{-1}	51.83 / 4.52×10^{-3}		-81.60
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + S + g$	0.967	0.919	29.29	0.59 / 6.63×10^{-1}	-1.53×10^{-4} / 2.45×10^{-2}	43.42 / 7.13×10^{-3}	-1.25 / 3.44×10^{-1}	6.41×10^{-2} / 2.47×10^{-6}	-1.54 / 8.14×10^{-1}	43.05 / 1.80×10^{-2}	18.82 / 9.00×10^{-2}	-70.39

The dependence table of normal boiling points (NBPs) of 28 tetratomic compounds. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group II (28 NBP's)				A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	g'	Intercept
Variables	R	Adj. R^2	SE	coeff	coeff	coeff	coeff	coeff	coeff	coeff	
				p-val	p-val	p-val	p-val	p-val	p-val	p-val	
A	0.803	0.631	57.09	2.52							51.96
				2.72×10^{-7}							
$A + \Gamma_s$	0.907	0.808	41.15	2.69	2.00×10^{-4}						-15.61
				2.59×10^{-10}	3.70×10^{-5}						
$A + \Gamma_s + P_{av}$	0.931	0.850	36.40	-.18	2.40×10^{-4}	31.67					60.74
				8.67×10^{-1}	1.64×10^{-6}	9.43×10^{-3}					
$A + \Gamma_s + P_{av} + L_{av}$	0.953	0.893	30.79	-3.66	2.55×10^{-4}	84.58	-8.19				172.36
				1.49×10^{-2}	6.19×10^{-8}	1.69×10^{-4}	3.57×10^{-3}				
$A + \Gamma_s + P_{av} + L_{av} + \Gamma m$	0.953	0.888	31.43	-3.36	2.29×10^{-4}	81.29	-7.65	5.62×10^{-3}			154.46
				7.02×10^{-2}	2.44×10^{-2}	1.46×10^{-3}	2.51×10^{-2}	7.75×10^{-1}			
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.954	0.884	32.03	-2.98	2.12×10^{-4}	77.20	-7.10	6.17×10^{-3}	2.79		129.96
				1.52×10^{-1}	5.80×10^{-2}	5.26×10^{-3}	5.48×10^{-2}	7.59×10^{-1}	6.80×10^{-1}		
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + g'$	0.955	0.881	32.40	-3.24	2.13×10^{-4}	81.68	-8.09	3.42×10^{-3}	4.55	9.65	122.78
				1.32×10^{-1}	6.00×10^{-2}	4.90×10^{-3}	4.52×10^{-2}	8.69×10^{-1}	5.33×10^{-1}	4.77×10^{-1}	

The dependence table of normal boiling points (NBPs) of 67 compounds (pentatomic compounds and some methane derivatives). The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group III (67 NBP's) Variables	R	Adj. R^2	SE	A coeff / p-val	Γ_s coeff / p-val	P_{av} coeff / p-val	L_{av} coeff / p-val	Γ_m coeff / p-val	$\sigma_{r,ep}$ coeff / p-val	Intercept
A	0.826	0.677	49.14	2.50 / 7.98×10^{-18}						17.29
$A + \Gamma_s$	0.903	0.809	37.81	2.76 / 1.01×10^{-24}	2.98×10^{-4} / 4.79×10^{-9}					-71.17
$A + \Gamma_s + P_{av}$	0.944	0.886	29.22	-.30 / 5.37×10^{-1}	2.44×10^{-4} / 2.12×10^{-9}	36.28 / 8.17×10^{-9}				17.87
$A + \Gamma_s + P_{av} + L_{av}$	0.970	0.936	21.95	-3.71 / 6.03×10^{-8}	1.74×10^{-4} / 5.09×10^{-8}	81.55 / 1.01×10^{-15}	-5.66 / 1.77×10^{-9}			178.67
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m$	0.974	0.944	20.37	-4.49 / 4.77×10^{-10}	4.36×10^{-5} / 3.61×10^{-1}	94.28 / 2.99×10^{-17}	-6.31 / 2.11×10^{-11}	3.20×10^{-2} / 1.51×10^{-3}		181.83
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.977	0.951	19.22	-4.27 / 4.42×10^{-10}	1.41×10^{-5} / 7.58×10^{-1}	91.95 / 1.18×10^{-17}	-6.05 / 1.74×10^{-11}	1.75×10^{-2} / 9.77×10^{-2}	9.55 / 4.88×10^{-3}	162.78

The dependence table of normal boiling points (NBPs) of 31 ethane and propane derivatives. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group IV (31 NBP's) Variables	R	Adj. R^2	SE	A coeff / p-val	Γ_s coeff / p-val	P_{av} coeff / p-val	L_{av} coeff / p-val	Γ_m coeff / p-val	$\sigma_{r,ep}$ coeff / p-val	Intercept
A	0.675	0.437	49.04	2.61 / 3.08×10^{-5}						25.73
$A + \Gamma_s$	0.832	0.671	37.51	1.67 / 9.98×10^{-4}	2.28×10^{-4} / 7.34×10^{-5}					52.01
$A + \Gamma_s + P_{av}$	0.852	0.696	36.05	-1.96 / 3.45×10^{-1}	2.63×10^{-4} / 1.98×10^{-5}	38.51 / 7.98×10^{-2}				168.14
$A + \Gamma_s + P_{av} + L_{av}$	0.879	0.737	33.52	-1.58 / 4.15×10^{-1}	1.93×10^{-4} / 2.09×10^{-3}	56.85 / 1.27×10^{-2}	-10.26 / 3.04×10^{-2}			227.57
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m$	0.969	0.926	17.79	-3.26 / 4.06×10^{-3}	3.31×10^{-5} / 3.63×10^{-1}	89.48 / 7.72×10^{-8}	-10.90 / 1.10×10^{-4}	6.29×10^{-2} / 1.49×10^{-8}		178.65
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.969	0.923	18.16	-3.27 / 5.00×10^{-3}	3.24×10^{-5} / 3.97×10^{-1}	89.76 / 2.22×10^{-7}	-10.94 / 1.69×10^{-4}	6.49×10^{-2} / 8.68×10^{-3}	-.73 / 9.29×10^{-1}	179.52

Table S6

The dependence table of critical temperatures (CTs) of 31 mono-, di- and triatomic compounds. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group I (31 CT's) Variables	R	Adj. R^2	SE	A coeff / p-val	Γ_s coeff / p-val	P_{av} coeff / p-val	L_{av} coeff / p-val	Γ_m coeff / p-val	$\sigma_{r,ep}$ coeff / p-val	S coeff / p-val	g coeff / p-val	Intercept
A	0.674	0.436	124.63	5.98 / 3.18×10^{-5}								-55.22
$A + \Gamma_s$	0.789	0.596	105.52	5.03 / 5.78×10^{-5}	5.16×10^{-4} / 1.46×10^{-3}							-52.52
$A + \Gamma_s + P_{av}$	0.815	0.627	101.29	-.98 / 7.77×10^{-1}	6.05×10^{-4} / 3.64×10^{-4}	71.97 / 7.68×10^{-2}						33.22
$A + \Gamma_s + P_{av} + L_{av}$	0.858	0.695	91.70	-6.52 / 9.35×10^{-2}	6.20×10^{-4} / 9.52×10^{-5}	143.73 / 3.45×10^{-3}	-9.71 / 1.40×10^{-2}					192.70
$A + \Gamma_s + P_{av} + L_{av} + \Gamma m$	0.937	0.852	63.74	1.97 / 5.24×10^{-1}	-1.67×10^{-4} / 3.47×10^{-1}	59.54 / 9.94×10^{-2}	-3.06 / 2.92×10^{-1}	9.44×10^{-2} / 1.44×10^{-5}				-80.86
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.938	0.849	64.53	1.43 / 6.59×10^{-1}	-1.78×10^{-4} / 3.24×10^{-1}	64.18 / 8.72×10^{-2}	-3.43 / 2.55×10^{-1}	8.24×10^{-2} / 4.37×10^{-3}	8.18 / 5.37×10^{-1}			-70.71
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + S$	0.944	0.859	62.28	0.38 / 9.06×10^{-1}	-1.95×10^{-4} / 2.67×10^{-1}	77.49 / 4.02×10^{-2}	-3.02 / 3.00×10^{-1}	8.23×10^{-2} / 3.46×10^{-3}	10.62 / 4.11×10^{-1}	61.30 / 1.10×10^{-1}		-73.21
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + S + g$	0.954	0.878	57.92	-1.13 / 7.11×10^{-1}	-2.12×10^{-4} / 1.96×10^{-1}	92.58 / 1.22×10^{-2}	-3.87 / 1.62×10^{-1}	1.01×10^{-1} / 5.64×10^{-4}	-8.51 / 5.71×10^{-1}	33.12 / 3.77×10^{-1}	57.64 / 4.34×10^{-2}	-55.64

The dependence table of critical temperatures (CTs) of 19 tetratomic compounds. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group II (19 CT's)				A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	g'	Intercept
Variables	R	Adj. R^2	SE	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	
A	0.764	0.559	87.67	3.56 / 1.40×10^{-4}							102.13
$A + \Gamma_s$	0.862	0.710	71.12	3.78 / 9.70×10^{-6}	4.32×10^{-4} / 6.38×10^{-3}						2.60
$A + \Gamma_s + P_{av}$	0.933	0.845	51.93	-2.33 / 1.75×10^{-1}	5.33×10^{-4} / 1.23×10^{-4}	72.86 / 1.50×10^{-3}					133.19
$A + \Gamma_s + P_{av} + L_{av}$	0.960	0.900	41.87	-7.82 / 3.70×10^{-3}	5.00×10^{-4} / 3.80×10^{-5}	156.45 / 2.14×10^{-4}	-12.05 / 9.32×10^{-3}				309.88
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m$	0.961	0.895	42.82	-6.96 / 2.24×10^{-2}	4.16×10^{-4} / 2.26×10^{-2}	147.46 / 1.12×10^{-3}	-10.46 / 4.93×10^{-2}	1.82×10^{-2} / 5.46×10^{-1}			255.63
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.963	0.891	43.62	-8.07 / 2.43×10^{-2}	4.88×10^{-4} / 2.57×10^{-2}	159.54 / 1.72×10^{-3}	-12.02 / 4.47×10^{-2}	1.42×10^{-2} / 6.48×10^{-1}	-7.92 / 4.81×10^{-1}		325.78
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + g'$	0.971	0.908	40.13	-9.17 / 9.92×10^{-3}	5.48×10^{-4} / 1.11×10^{-2}	177.34 / 6.73×10^{-4}	-16.37 / 1.27×10^{-2}	-7.27×10^{-4} / 9.81×10^{-1}	-3.94 / 7.08×10^{-1}	36.15 / 1.02×10^{-1}	319.52

Table S8

The dependence table of critical temperatures (CTs) of 42 compounds (pentatomic compounds and some methane derivatives). The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group III (42 CT's)				A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	Intercept
Variables	R	Adj. R^2	SE	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	
A	0.772	0.587	83.46	3.13 / 2.07×10^{-9}						103.79
$A + \Gamma_s$	0.895	0.791	59.36	3.72 / 6.32×10^{-15}	5.81×10^{-4} / 1.80×10^{-7}					-58.52
$A + \Gamma_s + P_{av}$	0.952	0.900	41.12	-1.59 / 6.44×10^{-2}	4.91×10^{-4} / 4.58×10^{-9}	65.75 / 9.18×10^{-8}				82.47
$A + \Gamma_s + P_{av} + L_{av}$	0.962	0.918	37.26	-5.59 / 7.21×10^{-4}	3.75×10^{-4} / 4.93×10^{-6}	121.08 / 6.99×10^{-7}	-7.19 / 4.26×10^{-3}			263.97
$A + \Gamma_s + P_{av} + L_{av} + \Gamma m$	0.967	0.926	35.40	-6.05 / 1.90×10^{-4}	1.99×10^{-4} / 6.08×10^{-2}	129.81 / 1.11×10^{-7}	-7.29 / 2.50×10^{-3}	4.32×10^{-2} / 3.18×10^{-2}		249.67
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.973	0.939	32.16	-5.79 / 1.05×10^{-4}	1.43×10^{-4} / 1.44×10^{-1}	126.89 / 2.94×10^{-8}	-6.71 / 2.36×10^{-3}	3.20×10^{-3} / 8.86×10^{-1}	21.08 / 5.82×10^{-3}	221.13

The dependence table of critical temperatures (CTs) of 23 ethane and propane derivatives. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group IV (23 CT's)				A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	Intercept
Variables	**R**	**Adj. R^2**	**SE**	coeff	coeff	coeff	coeff	coeff	coeff	
				p-val	p-val	p-val	p-val	p-val	p-val	
A	0.587	0.313	75.19	3.67						92.81
				3.24×10^{-3}						
$A + \Gamma_s$	0.888	0.767	43.83	1.68	4.03×10^{-4}					182.32
				2.88×10^{-2}	2.65×10^{-6}					
$A + \Gamma_s + P_{av}$	0.890	0.759	44.51	-.30	4.16×10^{-4}	23.97				225.55
				9.28×10^{-1}	5.42×10^{-6}	5.36×10^{-1}				
$A + \Gamma_s + P_{av} + L_{av}$	0.918	0.808	39.79	0.11	3.10×10^{-4}	49.20	-14.80			336.37
				9.71×10^{-1}	5.67×10^{-4}	1.83×10^{-1}	2.72×10^{-2}			
$A + \Gamma_s + P_{av} + L_{av} + \Gamma m$	0.958	0.893	29.68	-4.65	1.26×10^{-4}	126.39	-16.67	6.32×10^{-2}		336.49
				7.67×10^{-2}	1.00×10^{-1}	1.35×10^{-3}	2.16×10^{-3}	1.11×10^{-3}		
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.958	0.886	30.59	-4.61	1.28×10^{-4}	125.55	-16.61	5.94×10^{-2}	1.39	334.99
				9.35×10^{-2}	1.21×10^{-1}	2.73×10^{-3}	3.35×10^{-3}	2.42×10^{-1}	9.34×10^{-1}	

The dependence table of normal freezing points (NFPs) of 39 mono-, di- and triatomic compounds. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group I (39 NFP's)

Variables	R	Adj. R^2	SE	A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	S	g	Intercept
				coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	
A	0.603	0.347	65.51	2.46 / 4.83×10^{-5}								-2.80
$A + \Gamma_s$	0.788	0.600	51.24	2.04 / 2.94×10^{-5}	2.78×10^{-4} / 1.77×10^{-5}							-8.92
$A + \Gamma_s + P_{av}$	0.847	0.693	44.93	-2.50 / 7.70×10^{-2}	3.38×10^{-4} / 1.87×10^{-7}	51.04 / 1.52×10^{-3}						70.74
$A + \Gamma_s + P_{av} + L_{av}$	0.872	0.733	41.90	-4.54 / 5.11×10^{-3}	3.46×10^{-4} / 3.52×10^{-8}	80.90 / 9.45×10^{-5}	-4.65 / 1.75×10^{-2}					125.30
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m$	0.896	0.773	38.61	-2.60 / 1.10×10^{-1}	1.60×10^{-4} / 6.26×10^{-2}	61.37 / 2.10×10^{-3}	-3.10 / 9.65×10^{-2}	2.61×10^{-2} / 1.21×10^{-2}				58.22
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.902	0.779	38.10	-3.32 / 5.20×10^{-2}	1.45×10^{-4} / 9.05×10^{-2}	69.16 / 9.57×10^{-4}	-3.76 / 5.07×10^{-2}	1.12×10^{-2} / 4.45×10^{-1}	10.21 / 1.80×10^{-1}			68.43
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + S$	0.922	0.816	34.73	-3.86 / 1.59×10^{-2}	1.27×10^{-4} / 1.03×10^{-1}	76.42 / 1.33×10^{-4}	-3.39 / 5.42×10^{-2}	1.11×10^{-2} / 4.08×10^{-1}	12.68 / 7.32×10^{-2}	54.49 / 1.01×10^{-2}		59.08
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + S + g$	0.923	0.812	35.14	-4.20 / 1.71×10^{-2}	1.37×10^{-4} / 9.32×10^{-2}	80.21 / 2.28×10^{-4}	-3.60 / 4.97×10^{-2}	1.23×10^{-2} / 3.72×10^{-1}	10.73 / 1.82×10^{-1}	51.44 / 2.00×10^{-2}	7.01 / 6.05×10^{-1}	63.20

Table S11

The dependence table of normal freezing points (NFPs) of 28 tetratomic compounds. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group II (28 NFP's) Variables	R	Adj. R^2	SE	A coeff / p-val	Γ_s coeff / p-val	P_{av} coeff / p-val	L_{av} coeff / p-val	Γ_m coeff / p-val	$\sigma_{r,ep}$ coeff / p-val	g' coeff / p-val	Intercept
A	0.571	0.300	55.38	1.26 / 1.51×10^{-3}							73.88
$A + \Gamma_s$	0.783	0.583	42.75	1.42 / 2.71×10^{-5}	1.80×10^{-4} / 2.19×10^{-4}						13.31
$A + \Gamma_s + P_{av}$	0.822	0.636	39.95	-.98 / 4.00×10^{-1}	2.13×10^{-4} / 3.34×10^{-5}	26.49 / 4.18×10^{-2}					77.19
$A + \Gamma_s + P_{av} + L_{av}$	0.844	0.663	38.44	-3.28 / 7.18×10^{-2}	2.23×10^{-4} / 1.44×10^{-5}	61.31 / 1.59×10^{-2}	-5.39 / 1.01×10^{-1}				150.64
$A + \Gamma_s + P_{av} + L_{av} + \Gamma m$	0.850	0.659	38.66	-2.17 / 3.29×10^{-1}	1.29×10^{-4} / 2.82×10^{-1}	49.29 / 8.68×10^{-2}	-3.41 / 3.93×10^{-1}	2.05×10^{-2} / 3.99×10^{-1}			85.24
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.851	0.645	39.45	-2.55 / 3.14×10^{-1}	1.47×10^{-4} / 2.71×10^{-1}	53.48 / 9.45×10^{-2}	-3.97 / 3.67×10^{-1}	2.00×10^{-2} / 4.23×10^{-1}	-2.86 / 7.31×10^{-1}		110.29
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep} + g'$	0.861	0.651	39.10	-2.05 / 4.20×10^{-1}	1.44×10^{-4} / 2.76×10^{-1}	44.71 / 1.67×10^{-1}	-2.03 / 6.61×10^{-1}	2.54×10^{-2} / 3.16×10^{-1}	-6.31 / 4.75×10^{-1}	-18.90 / 2.54×10^{-1}	124.36

Table S12

The dependence table of normal freezing points (NFPs) of 58 compounds (tetratomic compounds and some methane derivatives). The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group III (58 NFP's) Variables	R	Adj. R^2	SE	A coeff / p-val	Γ_s coeff / p-val	P_{av} coeff / p-val	L_{av} coeff / p-val	Γ_m coeff / p-val	$\sigma_{r,ep}$ coeff / p-val	Intercept
A	0.786	0.610	38.48	1.61 / 2.84×10^{-13}						1.24
$A + \Gamma_s$	0.857	0.725	32.35	1.76 / 4.01×10^{-17}	2.02×10^{-4} / 8.13×10^{-6}					-54.46
$A + \Gamma_s + P_{av}$	0.885	0.770	29.55	0.03 / 9.49×10^{-1}	1.74×10^{-4} / 3.24×10^{-5}	20.53 / 1.08×10^{-3}				-5.50
$A + \Gamma_s + P_{av} + L_{av}$	0.908	0.810	26.84	-2.23 / 7.08×10^{-3}	1.26×10^{-4} / 1.33×10^{-3}	50.71 / 6.39×10^{-6}	-3.74 / 8.80×10^{-4}			98.45
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m$	0.920	0.832	25.24	-2.87 / 5.62×10^{-4}	-2.32×10^{-5} / 7.16×10^{-1}	61.93 / 1.90×10^{-7}	-4.17 / 1.31×10^{-4}	3.78×10^{-2} / 6.83×10^{-3}		92.80
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.925	0.839	24.74	-3.17 / 1.80×10^{-4}	-1.15×10^{-6} / 9.86×10^{-1}	65.45 / 5.78×10^{-8}	-4.60 / 3.72×10^{-5}	5.64×10^{-2} / 1.54×10^{-3}	-9.91 / 8.35×10^{-2}	113.18

Table S13

The dependence table of normal freezing points (NFPs) of 30 ethane and propane derivatives. The table shows the effect of successive addition of molecular descriptors as independent variables on the correlation parameters (R, adjusted R^2 and SE) in addition to the coefficients and p-values of the independent variables.

Group IV (30 NFP's)				A	Γ_s	P_{av}	L_{av}	Γ_m	$\sigma_{r,ep}$	Intercept
Variables	R	Adj. R^2	SE	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	coeff / p-val	
A	0.559	0.288	50.13	1.99 / 1.33×10^{-3}						-55.08
$A + \Gamma_s$	0.634	0.358	47.59	1.37 / 3.45×10^{-2}	1.31×10^{-4} / 5.37×10^{-2}					-29.78
$A + \Gamma_s + P_{av}$	0.678	0.398	46.09	-2.90 / 2.80×10^{-1}	1.67×10^{-4} / 1.85×10^{-2}	45.98 / 1.07×10^{-1}				102.61
$A + \Gamma_s + P_{av} + L_{av}$	0.864	0.705	32.24	-1.85 / 3.26×10^{-1}	1.72×10^{-5} / 7.56×10^{-1}	84.15 / 3.96×10^{-4}	-23.15 / 1.70×10^{-5}			238.50
$A + \Gamma_s + P_{av} + L_{av} + \Gamma m$	0.911	0.795	26.88	-3.25 / 5.26×10^{-2}	-9.66×10^{-5} / 9.81×10^{-2}	109.01 / 4.83×10^{-6}	-22.85 / 1.72×10^{-6}	4.27×10^{-2} / 2.03×10^{-3}		198.83
$A + \Gamma_s + P_{av} + L_{av} + \Gamma_m + \sigma_{r,ep}$	0.911	0.786	27.45	-3.27 / 5.73×10^{-2}	-9.82×10^{-5} / 1.07×10^{-1}	109.57 / 9.76×10^{-6}	-22.94 / 3.35×10^{-6}	4.71×10^{-2} / 1.84×10^{-1}	-1.66 / 8.93×10^{-1}	200.95

Figure S1

Figure S1: Experimental (X-axis) vs predicted (Y-axis) values of normal boiling points (NBPs) of Group I, II, III and IV compounds, where the full-variable relation is used<mark>, with the correlation coefficient (R) and the standard error (SE) depicted on the graphs</mark>
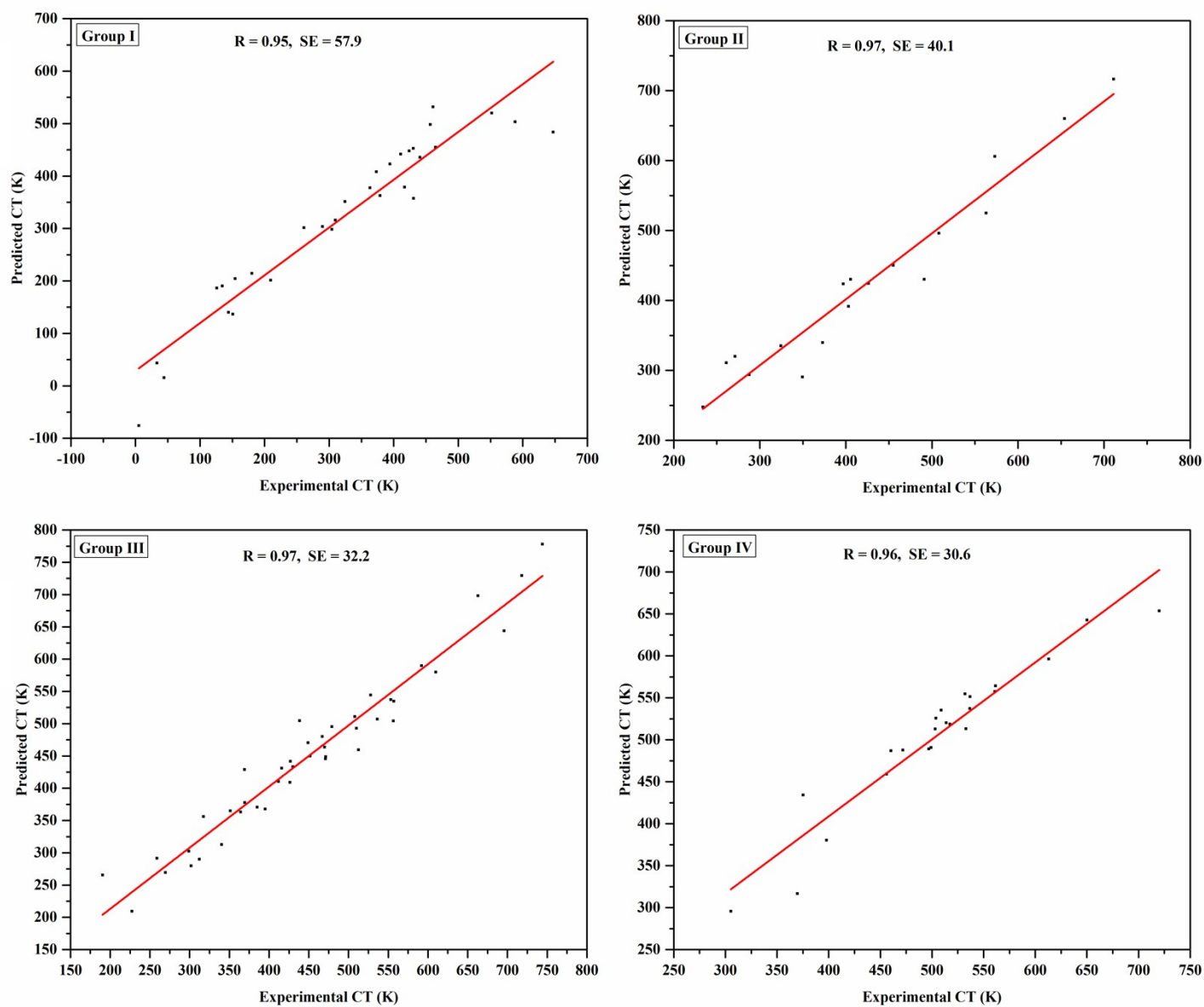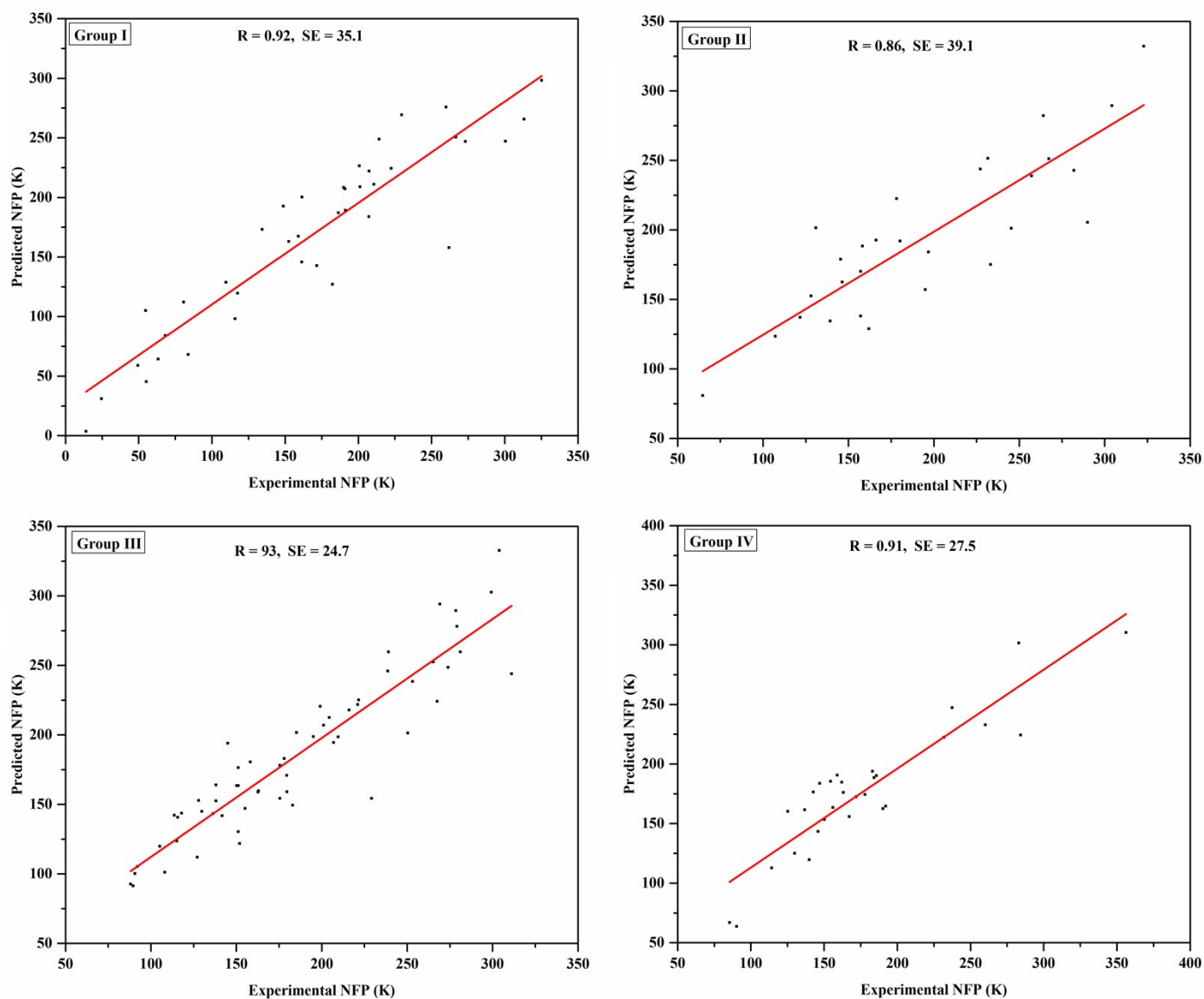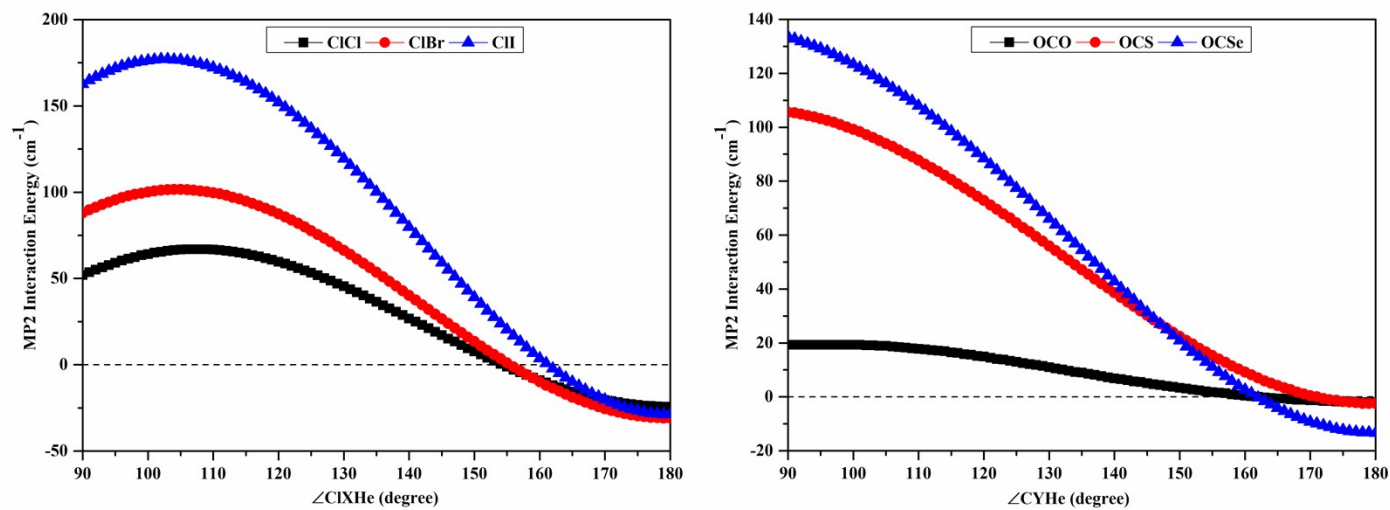
Figure S2

Figure S2: Experimental (X-axis) vs predicted (Y-axis) values of critical temperatures (CTs) of Group I, II, III and IV compounds, where the full-variable relation is used, with the correlation coefficient (R) and the standard error (SE) depicted on the graphs

Figure S3

Figure S3: Experimental (X-axis) vs predicted (Y-axis) values of normal freezing points (NFPs) of Group I, II, III and IV compounds, where the full-variable relation is used, with the correlation coefficient (R) and the standard error (SE) depicted on the graphs

Figure S4

Figure S4: The interaction energies of the of ClX⋯He and OCY⋯He complexes (X = Cl, Br and I and Y = O, S and Se) calculated at MP2/aug-cc-pVDZ level of theory, where the ∠ClXHe and ∠CYHe angles increase from 90° to 180° and the X/Y⋯He distance is the sum of the VdW radii of the X/Y and He atoms

Figure S5
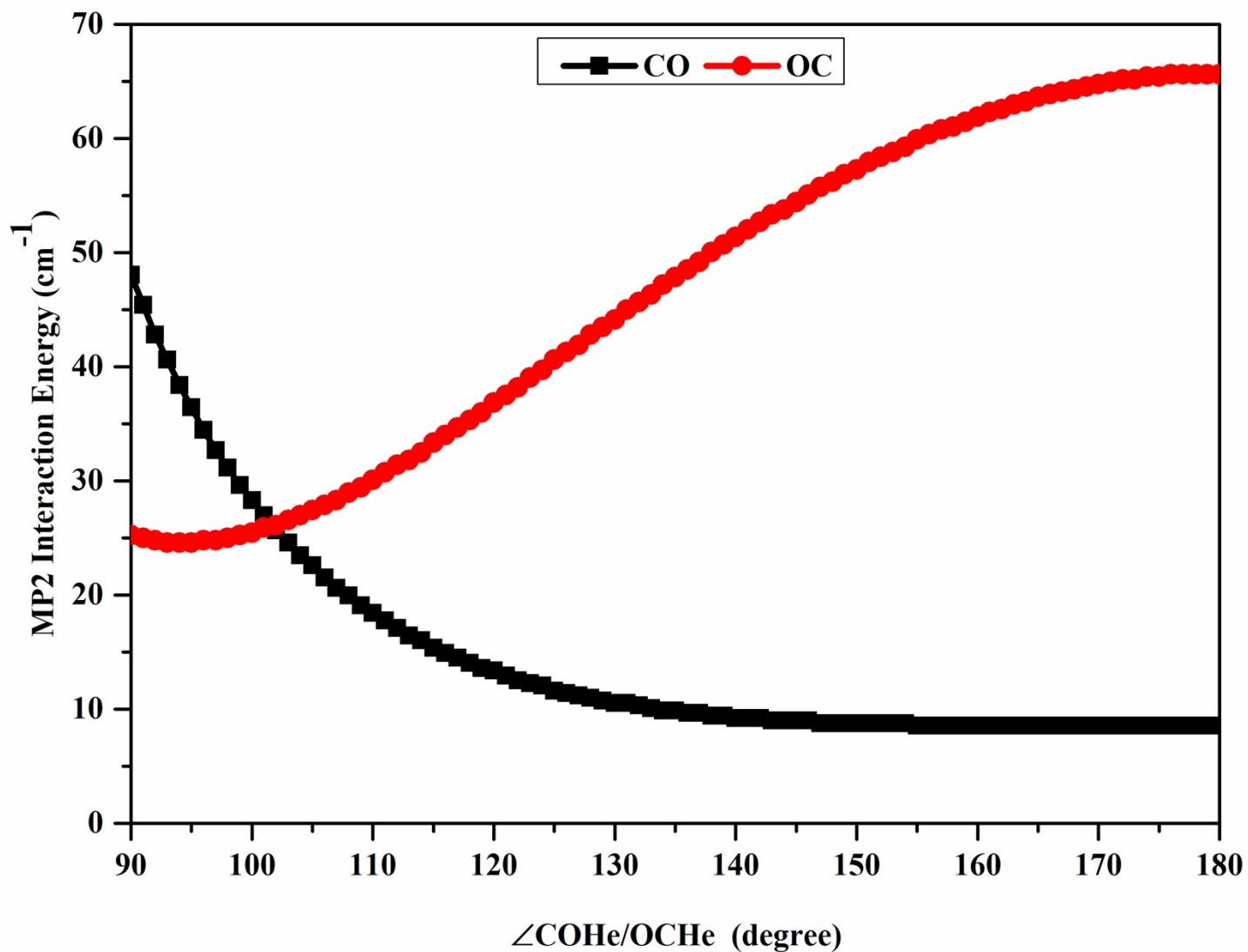
Figure S5: The interaction energies of the of CO···He and OC···He complexes calculated at MP2/aug-cc-pVDZ level of theory, where the ∠COHe and ∠OCHe angles increase from 90° to 180° and the C/O···He distance is the sum of the VdW radii of the C/O and He atoms
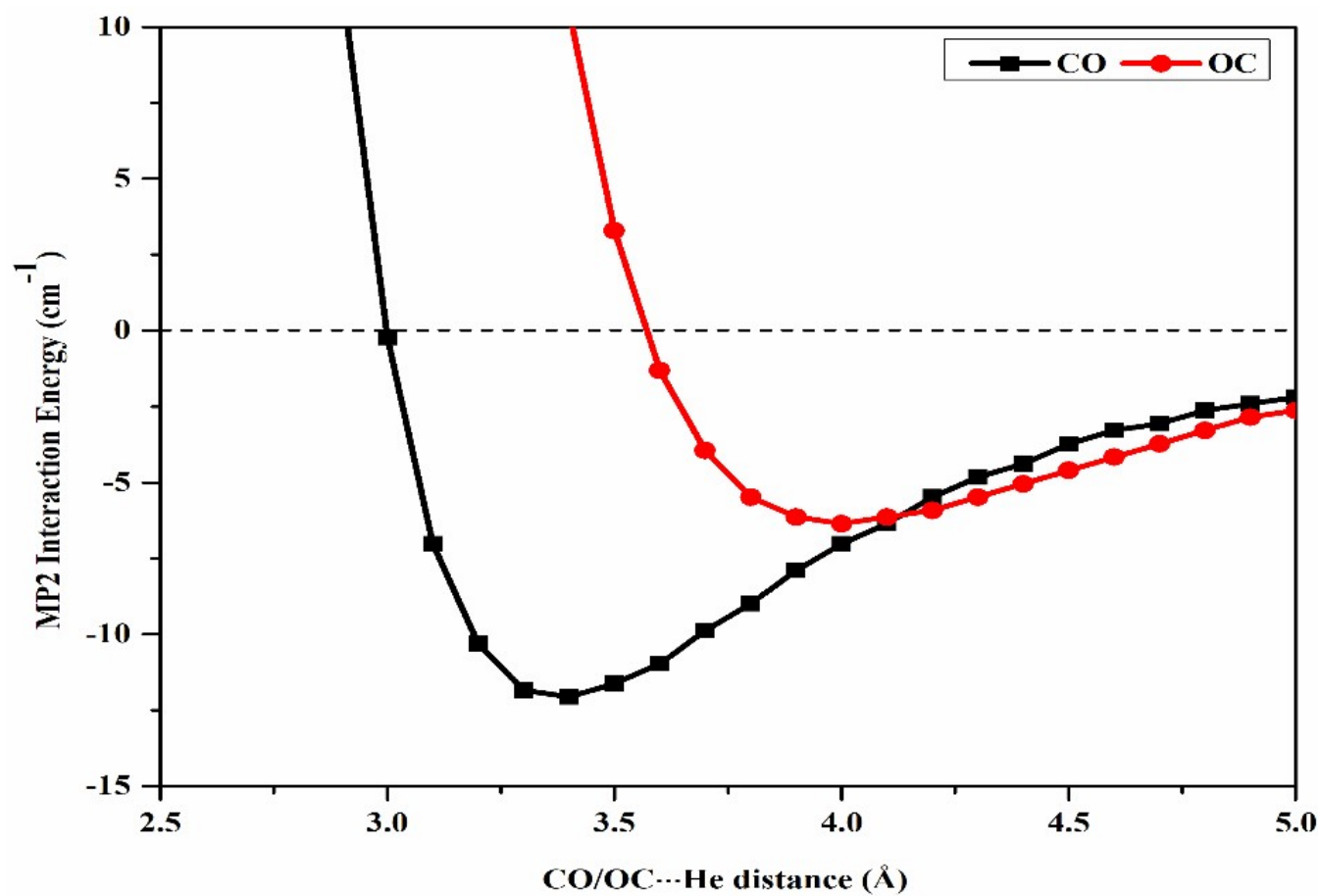
Figure S6: PES scan of the of CO/OC···He complexes calculated at MP2/aug-cc-pVDZ level of theory, where the ∠COHe and ∠COHe = 180° and the CO/OC···He distance ranged from 2.5 to 5 Å with a step size of 0.1 Å

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