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

Supporting Information: Signature of van der Waals Interactions in the Cumulant Density Matrix

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The square of the Frobenius norm as a function of distance for discussed dimer systems are provided in Tables S1 and S2, while the square of the Frobenius norm for the asymmetric molecules are in Table S3, respectively. Cartesian coordinates of the molecules in Tables 1 and 2 at 6 Å separation are given in Tables S4 through S13. All distances are in Angstroms.

Table S1: Square of the Frobenius norm for different dimer systems as a function of the separation between the monomers, which is listed in Angstroms.

Separation (Å)	F_2	NH_3	BH_3	CH_4
2	586.745722625	-	-	-
2.5	586.643867962	-	-	-
3	586.624863028	-	-	-
3.5	586.618125802	171.476081327	-	-
4	586.61586214	171.496740533	106.105170234	169.321419337
4.5	586.614888941	171.509105851	106.110450095	169.341382111
5	586.614388307	171.514212533	106.11318198	169.339463286
5.5	586.614111993	171.515968908	106.11447768	169.344806386
6	586.613950251	171.516655864	106.115065952	169.343988199
6.5	586.613851331	171.517042796	106.115351539	169.346518079
7	586.613788546	171.517306611	106.115508813	169.345542085
7.5	586.613747409	171.517505145	106.115604242	169.345290688
8	586.613719705	171.517660585	106.11566534	169.348263807
8.5	586.613700592	171.517785047	106.115705782	169.345552341
9	586.613687121	171.517886395	106.115733256	169.349250224
9.5	586.613677446	171.517970026	106.115752344	169.346497184
10	586.613670377	171.518039795	106.115765873	169.350048923
10.5	586.613665133	171.518098535	106.115775635	169.345757412
11	586.613661188	171.518148379	106.115782794	169.348063419
11.5	586.613658182	171.518190973	106.115788121	169.346195519
12	586.613655866	171.518227598	106.115792138	169.346922789
12.5	586.613654061	171.518259268	106.115795205	169.34980696
13	586.61365264	171.518286794	106.115797573	169.345811889
13.5	586.613651513	171.518310835	106.11579942	169.345848706
14	586.61365061	171.518331923	106.115800875	169.351574146
14.5	586.613649881	171.518350497	106.115802031	169.34666408
15	586.613649288	171.51836692	106.115802957	169.350516505
15.5	586.613648802	171.518381494	106.115803705	169.345870982
16	586.613648402	171.51839447	106.115804313	169.351472796
16.5	586.61364807	171.518406062	106.11580481	169.349000725
17	586.613647792	171.518416447	106.11580522	169.347611997
17.5	586.613647559	171.518425779	106.11580556	169.34588283
18	586.613647362	171.518434187	106.115805843	169.35146145
18.5	586.613647195	171.518441783	106.11580608	169.345886692
19	586.613647053	171.518448662	106.11580628	169.345888281
19.5	586.61364693	171.518454905	106.115806449	169.360094861
20	586.613646826	171.518460585	106.115806592	169.349739106

Table S2: Square of the Frobenius norm for different dimer systems as a function of the separation between the monomers, which is listed in Angstroms.

Separation (Å)	Ar	Be	CO_2	SO_2
4	597.224961931	20.4782061546	882.225573458	1907.16831281
4.5	597.230284365	20.4554364036	882.24811541	1907.23403537
5	597.233060514	20.4443639529	882.258704662	1907.26889574
5.5	597.234494191	20.4390910111	882.264094491	1907.28619804
6	597.235236453	20.4364155361	882.267055457	1907.29491803
6.5	597.235633631	20.4349180669	882.268799996	1907.29948721
7	597.235861109	20.4340156669	882.269882599	1907.30193029
7.5	597.235997534	20.4334666136	882.270579978	1907.30321647
8	597.236081836	20.433135035	882.27104291	1907.30385575
8.5	597.236135679	20.4329320086	882.271358283	1907.30412882
9	597.236171232	20.4328041117	882.271578092	1907.30419484
9.5	597.236195333	20.432719602	882.271734434	1907.30414575
10	597.236211995	20.4326618443	882.271847675	1907.30403522
10.5	597.236223701	20.432621388	882.271931046	1907.30389473
11	597.236232054	20.4325925008	882.271993339	1907.30374273
11.5	597.236238105	20.4325715396	882.272040512	1907.30347014
12	597.236242548	20.4325561114	882.272076676	1907.30344307
12.5	597.236245857	20.4325446078	882.272104711	1907.30330267
13	597.23624835	20.4325359279	882.272126671	1907.30317293
13.5	597.236250246	20.4325293063	882.272144037	1907.30305337
14	597.236251708	20.4325242037	882.272157891	1907.30294385
14.5	597.236252842	20.4325202345	882.272169034	1907.30284391
15	597.236253731	20.4325171198	882.272178064	1907.30275293
15.5	597.236254435	20.4325146557	882.272185436	1907.30267019
16	597.236254997	20.4325126913	882.272191492	1907.302595
16.5	597.236255447	20.4325111142	882.2721965	1907.30252665
17	597.236255809	20.4325098394	882.272200664	1907.30246449
17.5	597.236256107	20.4325088026	882.272204146	1907.30240792
18	597.236256346	20.4325079541	882.272207073	1907.30301815
18.5	597.236256547	20.432507256	882.272209544	1907.30230941
19	597.236256708	20.4325066787	882.272211642	1907.30226651
19.5	597.236256845	20.4325061986	882.27221343	1907.30288495
20	597.236256957	20.4325057977	882.272214959	1907.30219138

Table S3: Square of the Frobenius norm for asymmetric two-molecule systems as a function of their separation, which is provided in Angstroms.

Separation (Å)	Ar-CO_2	Ar-SO_2
5.5	734.172999621	1161.62212281
6	734.173279058	1161.62249637
6.5	734.173421869	1161.62268397
7	734.173503304	1161.62279002
7.5	734.173552192	1161.62285348
8	734.173582623	1161.62289291
8.5	734.173602153	1161.62291819
9	734.173615027	1161.62293485
9.5	734.173623718	1161.62294608
10	734.17362971	1161.62295383
10.5	734.17363392	1161.62295926
11	734.173636928	1161.62296315
11.5	734.173639112	1161.62296597
12	734.17364072	1161.62296805
12.5	734.173641919	1161.62296959
13	734.173642824	1161.62297076
13.5	734.173643514	1161.62297165
14	734.173644046	1161.62297234
14.5	734.173644461	1161.62297288
15	734.173644785	1161.6229733
15.5	734.173645042	1161.62297363
16	734.173645247	1161.62297389
16.5	734.173645412	1161.6229741
17	734.173645545	1161.62297428
17.5	734.173645653	1161.62297442
18	734.173645742	1161.62297453
18.5	734.173645815	1161.62297462
19	734.173645875	1161.6229747
19.5	734.173645925	1161.62297477
20	734.173645967	1161.62297482

Table S4: Geometry for F_2 dimer at 6 Å

Atom	x	y	z
F	0.0	0.0	1.4119
F	0.0	0.0	0.0
F	0.0	0.0	6.0
F	6.0	0.0	4.5881

Table S5: Geometry for Ar-CO_2 at 6 Å

Atom	x	y	z
Ar	0.0	0.0	0.0
C	6.0	0.0	0.0
O	6.0	0.0	1.1621
O	6.0	0.0	-1.1621

Table S6: Geometry for Ar-SO_2 at 6 Å

Atom	x	y	z
Ar	0.0	0.0	0.0
S	6.0	0.0	0.0
O	6.0	1.2371	.7215
O	6.0	-1.2371	.7215

Table S7: Geometry for the BH_3 dimer at 6 Å

Atom	x	y	z
H	0.0	-1.1900	0.0
H	1.0306	.5950	0.0
H	-1.0306	.5950	.7215
B	0.0	0.0	0.0
B	0.0	0.0	6.0
H	6.0	1.1900	6.0
H	1.0306	-.5950	6.0
H	-1.0306	-.5950	6.0

Table S8: Geometry for the Ar dimer at 6 Å

Atom	x	y	z
Ar	0.0	0.0	0.0
Ar	0.0	0.0	6.0

Table S9: Geometry for the CH_4 dimer at 6 Å

Atom	x	y	z
H	0.0	0.0	1.1
H	.898	0.0	-.634
H	.898	0.0	-.634
H	0.0	-.898	-.634
C	0.0	0.0	0.0
C	0.0	0.0	6.0
H	.898	0.0	6.634
H	0.0	.898	6.634
H	0.0	-.898	6.634
H	0.0	0.0	4.9

Table S10: Geometry for NH_3 at 6 Å

Atom	x	y	z
H	0.0	0.0	0.0
H	0.0	-.9377	-.3816
H	.8121	.4689	-.3816
N	-.8121	.4689	-.3816
N	0.0	0.0	6.3816
H	0.0	0.9377	6.3816
H	-.8121	-.4689	6.3816
H	.8121	-.4689	6.3816

Table S11: Geometry for the Be dimer at 6 Å

Atom	x	y	z
Be	0.0	0.0	0.0
Be	0.0	0.0	6.0

Table S12: Geometry for CO_2 dimer at 6 Å

Atom	x	y	z
C	0.0	0.0	0.0
O	0.0	0.0	1.1621
O	0.0	0.0	-1.1621
C	6.0	0.0	0.0
O	6.0	0.0	1.1621
O	6.0	0.0	-1.1621

Table S13: Geometry for SO_2 dimer at 6 Å

Atom	x	y	z
S	0.0	0.0	0.0
O	0.0	-1.2371	-.7215
O	0.0	1.2371	.7215
S	6.0	0.0	0.0
O	6.0	-1.2371	-.7215
O	6.0	1.2371	.7215