Xe· · ·OCS: Relatively straightforward?

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Supplementary Material

Additional supplemental files and archives in computer-readable form are available on Zenodo, see DOI: 10.5281/zenodo.3582270

1 Isotopic data

The fits for all measured isotopologues are found in Tables S1 (main isotopologue of OCS) and S2 (minor isotopologues of OCS).

2 Transition list

Transitions are listed for each isotope as they are used in the fits in Tables S3-S11. Line uncertainties are assumed to be 2 kHz for all transitions. Transition quantum numbers are defined as $J''_{K''_a K''_c} \leftarrow J'_{K'_a K'_c}$. For the ^{131}Xe species, the nuclear spin couples to the molecular rotation and requires an additional quantum number. The spin, ($^{131}I = 3/2$) uses the following coupling scheme.

$$J + I = F \tag{1}$$

Where F becomes the additional quantum number needed to describe energy levels with quadrupolar coupling. This labeling is used only for Table S5.

3 Binding energies

Table S12 shows the binding energies D_E obtained using the Lennard-Jones model with R_{cm} derived from r_0 and r_e^{SE} structures, the associated rotational constants (B_0's and B_e^{SE}'s, respectively), and the experimental centrifugal distortion constant D_J, are compared to the results of the Lennard-Jones model applied to B2PLYP results (r_e^{B2PLYP}, B_e^{B2PLYP}, D_J^{B2PLYP}), as well as the results of the supermolecular approach using B2PLYP and MP2+δ(T).

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Table S1: Spectroscopic fits for the observed xenon isotopologues with the main carbonyl sulfide isotopic species, $^{16}O^{12}C^{32}S$.

		$^{16}O^{12}C^{32}S$					
		^{129}Xe	^{130}Xe	^{131}Xe	^{132}Xe	^{134}Xe	^{136}Xe
A	(MHz)	6556.08768(39)	6555.92026(20)	6555.75286(34)	6555.58843(43)	6555.26598(21)	6554.95134(29)
B	(MHz)	776.290440(85)	774.42305(34)	772.577500(66)	770.764639(77)	767.21410(12)	763.762671(99)
C	(MHz)	691.765215(87)	690.278972(45)	688.810688(40)	687.367332(40)	684.538365(91)	681.790073(91)
D_J	(kHz)	1.68469(93)	1.67613(69)	1.67679(44)	1.67077(35)	1.6568(13)	1.6709(11)
D_{JK}	(kHz)	20.843(17)	20.748(35)	20.6724(68)	20.6002(53)	20.3977(91)	[20.6002]
D_K	(kHz)	[105.409]	[105.409]	105.487(64)	105.409(95)	[105.409]	[105.409]
d_1	(kHz)	[-0.21153]	[-0.21153]	-0.21249(16)	-0.21153(15)	-0.20943(55)	[-0.21153]
d_2	(kHz)	[-0.03762]	[-0.03762]	-0.03859(27)	-0.03762(14)	[-0.03762]	[-0.03762]
χ_{aa}	(MHz)	-	-	-0.8765(21)	-	-	-
χ_{bb}	(MHz)	-	-	0.5793(23)	-	-	-
χ_{cc}	(MHz)	-	-	0.2973(32)	-	-	-
N		11	9	131	37	21	6
rms	(kHz)	0.8	0.2	1.6	0.8	0.9	0.3

Table S2: Spectroscopic fits for the observed xenon isotopologues with the minor isotopes of carbonyl sulfide.

		$^{16}O^{12}C^{32}S$	$^{16}O^{12}C^{34}S$		$^{16}O^{13}C^{32}S$
		^{132}Xe	^{129}Xe	^{132}Xe	^{132}Xe
A	(MHz)	6555.58843(43)	6422.9514(10)	6422.42070(27)	6526.7428(18)
B	(MHz)	770.764639(77)	755.99303(36)	750.49215(12)	763.03301(57)
C	(MHz)	687.367332(40)	674.14110(18)	669.757437(71)	680.89375(32)
D_J	(kHz)	1.67077(35)	1.6208(24)	1.5946(27)	1.6408(70)
D_{JK}	(kHz)	20.6002(53)	18.518(11)	18.261(11)	20.320(65)
D_K	(kHz)	105.409(95)	109.22(26)	109.284(61)	104.20(40)
d_1	(kHz)	-0.21153(15)	-0.20787(89)	-0.2024(11)	-0.2103(19)
d_2	(kHz)	-0.03762(14)	-0.0351(12)	-0.03252(97)	-0.0324(28)
N		37	15	21	14
rms	(kHz)	0.8	0.4	0.4	0.6

Table S3: Transition list for $^{132}Xe \cdots {}^{16}O^{12}C^{32}S$. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
1	1	0	1	0	1	5868.0734	-0.0002
2	1	1	2	0	2	5952.2771	0.0000
3	1	2	3	0	3	6080.2440	0.0002
8	2	6	9	1	9	6458.1073	0.0005
1	1	1	0	0	0	7242.8026	-0.0007
7	2	5	8	1	8	7453.3859	-0.0010
2	1	2	1	0	1	8617.4149	-0.0007
4	2	3	5	1	4	9567.5076	-0.0006
5	2	3	6	1	6	9646.0692	0.0014
3	1	3	2	0	2	9950.5617	-0.0008
7	0	7	6	0	6	10154.8913	0.0004
4	2	2	5	1	5	10831.3126	0.0013
4	1	4	3	0	3	11243.3486	-0.0006
8	1	8	7	1	7	11311.0090	0.0013
8	0	8	7	0	7	11587.3997	0.0008
8	2	7	7	2	6	11649.4642	-0.0024
8	2	6	7	2	5	11723.5403	0.0009
11	0	11	10	1	10	11972.8980	-0.0006
8	1	7	7	1	6	11975.8237	0.0005
3	2	1	4	1	4	12069.0114	0.0008
5	1	5	4	0	4	12497.5699	-0.0004
6	1	6	5	0	5	13715.7101	0.0002
7	1	7	6	0	6	14900.9315	0.0003
10	2	8	10	1	9	15661.4233	-0.0006
9	2	7	9	1	8	15920.0573	0.0000
8	1	8	7	0	7	16057.0493	0.0014
8	2	6	8	1	7	16179.5622	0.0000
7	2	5	7	1	6	16431.8459	0.0001
6	2	4	6	1	5	16669.4652	0.0002
5	2	3	5	1	4	16885.7564	0.0003
4	2	2	4	1	3	17074.9269	-0.0003
9	1	9	8	0	8	17188.4701	0.0013
3	2	1	3	1	2	17232.1156	-0.0005
2	2	0	2	1	1	17353.4210	-0.0003
2	2	1	1	1	0	20352.0460	-0.0006
2	2	0	1	1	1	20436.3350	-0.0006
12	1	12	11	0	11	20485.3850	-0.0007

Table S4: Transition list for $^{129}Xe \cdots {}^{16}O^{12}C^{32}S$. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
7	1	6	7	0	7	7092.3026	-0.0003
7	1	7	6	1	6	9966.5590	0.0011
7	0	7	6	0	6	10222.9513	-0.0012
3	2	2	4	1	3	11172.1224	-0.0014
5	1	5	4	0	4	12534.4561	-0.0002
6	1	6	5	0	5	13759.4335	-0.0005
7	1	7	6	0	6	14951.1782	-0.0005
8	1	8	7	0	7	16113.6091	-0.0002
4	2	2	4	1	3	17056.3086	0.0002
3	2	1	3	1	2	17215.4787	0.0016
9	1	9	8	0	8	17251.2534	0.0005

Table S5: Transition list for ^{131}Xe$\cdots$^{16}O^{12}C^{32}S. Frequency are in units of MHz.

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	Frequency	Obs-Calc
4	1	3	9/2	4	0	4	9/2	6254.3268	0.0003
4	1	3	7/2	4	0	4	7/2	6254.3880	0.0005
4	1	3	11/2	4	0	4	11/2	6254.5009	0.0005
4	1	3	5/2	4	0	4	5/2	6254.5620	0.0006
5	1	4	11/2	5	0	5	11/2	6477.4368	0.0005
5	1	4	9/2	5	0	5	9/2	6477.4901	0.0002
5	1	4	13/2	5	0	5	13/2	6477.6270	0.0007
5	1	4	7/2	5	0	5	7/2	6477.6806	0.0006
8	0	8	17/2	7	1	7	15/2	6872.4678	0.0002
8	0	8	15/2	7	1	7	13/2	6872.4980	0.0006
8	0	8	19/2	7	1	7	17/2	6872.6351	0.0002
8	0	8	13/2	7	1	7	11/2	6872.6654	0.0006
7	1	6	13/2	7	0	7	13/2	7082.9908	-0.0003
7	1	6	17/2	7	0	7	17/2	7083.1612	0.0000
7	1	6	11/2	7	0	7	11/2	7083.2048	0.0000
5	1	5	11/2	4	1	4	9/2	7092.6909	-0.0003
5	1	5	9/2	4	1	4	7/2	7092.6949	0.0001
5	1	5	13/2	4	1	4	11/2	7092.7006	0.0001
5	1	5	7/2	4	1	4	5/2	7092.7044	0.0005
1	1	1	1/2	0	0	0	3/2	7244.1056	0.0005
1	1	1	5/2	0	0	0	3/2	7244.3494	-0.0002
1	1	1	3/2	0	0	0	3/2	7244.6549	-0.0006
5	0	5	7/2	4	0	4	5/2	7288.0618	0.0003
5	0	5	9/2	4	0	4	7/2	7288.0684	0.0000
5	0	5	13/2	4	0	4	11/2	7288.0776	0.0000
5	0	5	11/2	4	0	4	9/2	7288.0846	0.0000
5	2	4	11/2	4	2	3	9/2	7303.2684	0.0058
5	2	4	9/2	4	2	3	7/2	7303.2750	0.0064
5	2	4	13/2	4	2	3	11/2	7303.2962	-0.0090
5	2	4	7/2	4	2	3	5/2	7303.3026	-0.0087
5	2	3	11/2	4	2	2	9/2	7321.2474	-0.0002
5	2	3	9/2	4	2	2	7/2	7321.2550	0.0000
5	2	3	13/2	4	2	2	11/2	7321.2975	0.0000
5	2	3	7/2	4	2	2	5/2	7321.3050	0.0002
5	1	4	9/2	4	1	3	7/2	7511.1706	-0.0002
5	1	4	7/2	4	1	3	5/2	7511.1819	0.0018
5	1	4	11/2	4	1	3	9/2	7511.1930	-0.0013
5	1	4	13/2	4	1	3	11/2	7511.2040	0.0005
9	0	9	19/2	8	1	8	17/2	8578.4236	-0.0001
9	0	9	17/2	8	1	8	15/2	8578.4478	-0.0006
9	0	9	21/2	8	1	8	19/2	8578.5793	0.0004

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Table S5 – *Continued from previous page*

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	Frequency	Obs-Calc
2	1	2	1/2	1	0	1	1/2	8621.6032	-0.0004
2	1	2	3/2	1	0	1	1/2	8621.6900	-0.0002
2	1	2	7/2	1	0	1	5/2	8621.8428	0.0020
2	1	2	5/2	1	0	1	5/2	8621.9269	-0.0006
2	1	2	1/2	1	0	1	3/2	8621.9986	0.0006
2	1	2	3/2	1	0	1	3/2	8622.0849	0.0001
2	1	2	5/2	1	0	1	3/2	8622.1466	0.0000
6	0	6	9/2	5	0	5	7/2	8735.3953	0.0041
6	0	6	11/2	5	0	5	9/2	8735.3993	-0.0002
6	0	6	15/2	5	0	5	13/2	8735.4027	0.0005
6	0	6	13/2	5	0	5	11/2	8735.4110	0.0003
3	1	3	3/2	2	0	2	1/2	9957.5173	-0.0008
3	1	3	9/2	2	0	2	7/2	9957.6873	-0.0006
3	1	3	7/2	2	0	2	7/2	9957.7193	-0.0013
3	1	3	3/2	2	0	2	3/2	9957.7356	0.0012
3	1	3	5/2	2	0	2	3/2	9957.7664	-0.0007
3	1	3	7/2	2	0	2	5/2	9957.9364	-0.0005
16	1	15	33/2	15	2	14	31/2	11150.2542	-0.0013
16	1	15	31/2	15	2	14	29/2	11150.2717	0.0012
4	1	4	5/2	3	0	3	3/2	11252.9004	-0.0012
4	1	4	11/2	3	0	3	9/2	11253.0039	-0.0009
4	1	4	7/2	3	0	3	5/2	11253.1254	-0.0004
4	1	4	9/2	3	0	3	7/2	11253.2285	-0.0005
5	1	5	7/2	4	0	4	5/2	12509.5290	-0.0001
5	1	5	13/2	4	0	4	11/2	12509.6018	-0.0005
5	1	5	9/2	4	0	4	7/2	12509.7375	-0.0009
5	1	5	11/2	4	0	4	9/2	12509.8113	-0.0003
6	1	6	9/2	5	0	5	7/2	13729.9305	-0.0007
6	1	6	15/2	5	0	5	13/2	13729.9877	0.0005
6	1	6	11/2	5	0	5	9/2	13730.1279	-0.0013
6	1	6	13/2	5	0	5	11/2	13730.1856	0.0005
7	1	7	11/2	6	0	6	9/2	14917.3069	0.0001
7	1	7	17/2	6	0	6	15/2	14917.3515	0.0003
7	1	7	13/2	6	0	6	11/2	14917.4948	0.0000
7	1	7	15/2	6	0	6	13/2	14917.5394	0.0001
8	1	8	13/2	7	0	7	11/2	16075.5066	0.0002
8	1	8	19/2	7	0	7	17/2	16075.5432	0.0004
8	1	8	15/2	7	0	7	13/2	16075.6850	0.0004
8	1	8	17/2	7	0	7	15/2	16075.7214	0.0003
7	2	5	11/2	7	1	6	11/2	16423.2860	0.0000
7	2	5	17/2	7	1	6	17/2	16423.3246	0.0000
7	2	5	13/2	7	1	6	13/2	16423.4748	-0.0005

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Table S5 – *Continued from previous page*

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	Frequency	Obs-Calc
7	2	5	15/2	7	1	6	15/2	16423.5137	-0.0002
6	2	4	9/2	6	1	5	9/2	16661.6835	0.0003
6	2	4	15/2	6	1	5	15/2	16661.7332	0.0000
6	2	4	11/2	6	1	5	11/2	16661.8999	0.0049
6	2	4	13/2	6	1	5	13/2	16661.9449	0.0000
5	2	3	7/2	5	1	4	7/2	16878.7447	-0.0007
5	2	3	13/2	5	1	4	13/2	16878.8127	-0.0003
5	2	3	9/2	5	1	4	9/2	16878.9843	-0.0009
5	2	3	11/2	5	1	4	11/2	16879.0523	-0.0006
4	2	2	5/2	4	1	3	5/2	17068.6208	0.0001
4	2	2	11/2	4	1	3	11/2	17068.7191	0.0001
4	2	2	9/2	4	1	3	7/2	17068.8658	-0.0003
4	2	2	7/2	4	1	3	7/2	17068.9012	0.0000
4	2	2	9/2	4	1	3	9/2	17068.9994	0.0000
9	1	9	15/2	8	0	8	13/2	17208.9795	0.0009
9	1	9	21/2	8	0	8	19/2	17209.0096	0.0009
9	1	9	17/2	8	0	8	15/2	17209.1477	0.0008
9	1	9	19/2	8	0	8	17/2	17209.1779	0.0008
3	2	1	3/2	3	1	2	3/2	17226.3770	0.0002
3	2	1	9/2	3	1	2	9/2	17226.5415	0.0002
3	2	1	5/2	3	1	2	5/2	17226.7297	0.0004
3	2	1	7/2	3	1	2	7/2	17226.8938	0.0000
3	2	2	7/2	3	1	3	7/2	17724.6648	0.0007
3	2	2	5/2	3	1	3	5/2	17724.6797	0.0003
3	2	2	9/2	3	1	3	9/2	17724.6976	0.0008
3	2	2	3/2	3	1	3	3/2	17724.7124	0.0002
10	1	10	17/2	9	0	9	15/2	18322.6790	0.0008
10	1	10	23/2	9	0	9	21/2	18322.7041	0.0007
10	1	10	19/2	9	0	9	17/2	18322.8370	0.0008
10	1	10	21/2	9	0	9	19/2	18322.8619	0.0004
11	1	11	19/2	10	0	10	17/2	19421.9354	0.0007
11	1	11	25/2	10	0	10	23/2	19421.9562	0.0004
11	1	11	21/2	10	0	10	19/2	19422.0819	0.0000
11	1	11	23/2	10	0	10	21/2	19422.1029	-0.0001
2	2	1	1/2	1	1	0	1/2	20353.6748	0.0002
2	2	1	3/2	1	1	0	1/2	20353.8925	-0.0011
2	2	1	7/2	1	1	0	5/2	20353.9009	0.0005
2	2	1	3/2	1	1	0	3/2	20354.0502	0.0005
2	2	1	5/2	1	1	0	5/2	20354.1194	0.0000
2	2	1	5/2	1	1	0	3/2	20354.2067	0.0005
12	1	12	21/2	11	0	11	19/2	20512.2776	-0.0007
12	1	12	27/2	11	0	11	25/2	20512.2950	-0.0012

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J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	Frequency	Obs-Calc
12	1	12	23/2	11	0	11	21/2	20512.4137	-0.0007
12	1	12	25/2	11	0	11	23/2	20512.4309	-0.0014
4	2	3	5/2	3	1	2	3/2	23065.6932	-0.0019
4	2	3	11/2	3	1	2	9/2	23065.8313	-0.0012
4	2	3	7/2	3	1	2	5/2	23065.9667	-0.0012
4	2	3	9/2	3	1	2	7/2	23066.1040	-0.0012

Table S6: Transition list for ^{134}Xe$\cdots$^{16}O^{12}C^{32}S. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
3	1	2	3	0	3	6080.8768	-0.0030
3	1	3	2	0	2	9936.4538	0.0002
4	1	4	3	0	3	11224.2752	0.0001
5	1	5	4	0	4	12473.8340	-0.0002
6	1	6	5	0	5	13687.5713	0.0001
9	2	7	9	1	8	15939.2487	0.0000
8	1	8	7	0	7	16020.6468	0.0000
7	2	5	7	1	6	16448.3778	0.0001
5	2	3	5	1	4	16899.1673	0.0003
4	2	2	4	1	3	17086.8814	0.0005
3	2	1	3	1	2	17242.8008	0.0003
3	2	2	3	1	3	17734.4026	0.0005
4	2	3	4	1	4	17900.2759	-0.0006
2	2	1	1	1	0	20348.2549	-0.0002
2	2	0	1	1	1	20431.8066	-0.0001
3	2	2	2	1	1	21716.8084	0.0000
3	2	1	2	1	2	21969.2073	0.0001
4	2	3	3	1	2	23043.6718	0.0000
4	2	2	3	1	3	23552.8142	0.0006
5	2	4	4	1	3	24328.9077	-0.0019
5	2	3	4	1	4	25186.1251	0.0012

Table S7: Transition list for ^{136}Xe$\cdots$^{16}O^{12}C^{32}S. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
4	1	4	3	0	3	11205.7336	0.0002
6	1	6	5	0	5	13660.2123	-0.0004
7	1	7	6	0	6	14837.1484	0.0002
7	2	5	7	1	6	16464.4246	0.0001
6	2	4	6	1	5	16698.9644	-0.0002
4	2	2	4	1	3	17098.4827	0.0000

Table S8: Transition list for ^{130}Xe$\cdots$^{16}O^{12}C^{32}S. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
1	1	1	0	0	0	7246.0461	-0.0003
2	1	2	1	0	1	8626.4813	0.0000
3	1	3	2	0	2	9965.0832	0.0001
4	1	4	3	0	3	11262.9780	0.0000
5	1	5	4	0	4	12521.9944	0.0002
6	1	6	5	0	5	13744.6617	-0.0002
5	2	3	5	1	4	16871.9292	-0.0001
4	2	2	4	1	3	17062.6045	0.0001
9	1	9	8	0	8	17230.0433	0.0000

Table S9: Transition list for $^{132}Xe \cdots {}^{16}O^{12}C^{34}S$. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
1	1	0	1	0	1	5752.5160	-0.0006
2	1	1	2	0	2	5834.0279	0.0002
3	1	2	3	0	3	5957.8828	0.0003
1	1	1	0	0	0	7092.0269	0.0001
2	1	2	1	0	1	8431.4301	-0.0003
3	1	3	2	0	2	9730.6933	0.0005
4	1	4	3	0	3	10990.8692	-0.0009
5	1	5	4	0	4	12213.6783	0.0005
6	1	6	5	0	5	13401.4897	-0.0003
7	1	7	6	0	6	14557.3318	0.0006
8	1	8	7	0	7	15684.8479	-0.0003
6	2	4	6	1	5	16351.9109	0.0001
5	2	3	5	1	4	16561.6537	0.0001
4	2	2	4	1	3	16744.9748	-0.0007
3	2	1	3	1	2	16897.2275	0.0000
2	2	0	2	1	1	17014.6805	0.0004
2	2	1	1	1	0	19934.9292	0.0000
2	2	0	1	1	1	20016.5164	0.0000
3	2	1	2	1	2	21520.4265	-0.0001
4	2	3	3	1	2	22572.3058	0.0001
4	2	2	3	1	3	23069.4531	-0.0001

Table S10: Transition list for $^{129}Xe \cdots {}^{16}O^{12}C^{34}S$. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
5	1	5	4	0	4	12250.4940	0.0009
6	1	6	5	0	5	13445.1300	0.0004
4	1	4	3	0	3	11020.4593	-0.0007
7	1	7	6	0	6	14607.4801	-0.0002
8	1	8	7	0	7	15741.2957	-0.0002
9	1	9	8	0	8	16850.9109	0.0000
3	1	3	2	0	2	9752.5868	-0.0005
3	2	1	3	1	2	16880.7713	0.0001
3	2	2	3	1	3	17367.4251	-0.0001
5	2	3	5	1	4	16540.9773	0.0000
5	2	4	5	1	5	17737.5176	-0.0001
4	2	3	4	1	4	17531.6983	0.0003
6	1	5	6	0	6	6614.0614	-0.0003
5	1	4	5	0	5	6345.4389	0.0005
4	1	3	4	0	4	6127.4442	0.0000

Table S11: Transition list for ^{132}Xe$\cdots$^{16}O^{13}C^{32}S. Frequency are in units of MHz.

J''	K_a''	K_c''	J'	K_a'	K_c'	Frequency	Obs-Calc
3	1	3	2	0	2	9889.9762	-0.0005
4	1	4	3	0	3	11171.0342	0.0010
5	1	5	4	0	4	12414.0691	-0.0001
6	1	6	5	0	5	13621.5033	-0.0005
7	1	7	6	0	6	14796.4176	0.0001
8	1	8	7	0	7	15942.5254	0.0000
2	2	1	1	1	0	20259.0615	0.0000
2	2	0	1	1	1	20342.0687	-0.0004
3	2	2	2	1	1	21620.3276	-0.0001
3	2	1	2	1	2	21871.0810	0.0011
4	2	3	3	1	2	22940.1748	0.0000
4	2	2	3	1	3	23445.9846	-0.0011
5	2	4	4	1	3	24218.6655	0.0000
5	2	3	4	1	4	25070.2547	0.0003

Table S12: Binding energies for the studied complexes, obtained from the Lennard-Jones model using experimental r_0 structures and distortion constants, semi-experimental r_e^{SE} structures and experimental distortion constants, calculated r_e^{B2PLYP} structures and distortion constants. The binding energies obtained using the supermolecular approach with B2PLYP and MP2+δ(T) are included for comparison.

Complex	D_E (kJ/mol)				
	Lennard-Jones			Supermolecular	
	r_0	r_e^{SE}	r_e^{B2PLYP}	B2PLYP	MP2+δ(T)
He$\cdots$OCS	-0.152	-0.119	-0.551	0.075	-0.035
Ne$\cdots$OCS	-0.518	-0.499	-1.535	-0.270	-0.381
Ar$\cdots$OCS	-1.943	-1.977	-3.866	-1.764	-2.007
Kr$\cdots$OCS	-2.536	-2.508	-3.043	-2.551	-2.871
Xe$\cdots$OCS	-3.158	-3.138	-3.906	-3.827	-3.827
Hg$\cdots$OCS	-3.157	-3.125	-4.484	-5.336	-4.148