Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

Versatile Interactions of Boron Fullerene B-80 with Gas Molecules

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Table S1. Geometric parameters of the gas molecules (X) in vacuum and their complexes with the boronfullerene, $X@B_{80}$. Distances are in angstroms, angles and dihedrals are in degrees.

Parameter	CO_2	$CO_2@B_{80}$	Parameter	H_2S	$H_2S@B_{80}$
R(C-O)	1.1828	1.1824	R(H-S)	1.3669	1.3732
R(C-O)	1.1828	1.1814	R(H-S)	1.3669	1.3667
A(O-C-O)	180.00	178.65	A(H-S-H)	92.74	92.28
Parameter	H_2	$H_2@B_{80}$	Parameter	HF	$HF@B_{80}$
R(H-H)	0.7480	0.7492	R(H-F)	0.9402	0.9455
Parameter	SO_2	$SO_2@B_{80}$	Parameter	NH_3	$NH_3@B_{80}$
R(S-O)	1.4704	1.4762	R(H-N)	1.0260	1.0333
R(O-S-O)	119.97	118.83	A(H-N-H)	106.87	108.15
			D(N-H-H-H)	-38.88	-37.05

Table S2. Boron-boron bond length alteration due to formation of $X@B_{80}$ complexes: $\Delta R(B\text{-}B) = R_{B\text{-}B}(B_{80}) - R_{B\text{-}B}(X@B_{80})$. X = {$CO_2$; H_2; H_2S; HF; NH_3; SO_2}. Compare changes in the $NH_3@B_{80}$ complex to other cases.

ΔR (B-B)	Gas molecules					
	$CO_2@B_{80}$	$H_2@B_{80}$	$H_2S@B_{80}$	$HF@B_{80}$	$NH_3@B_{80}$	$SO_2@B_{80}$
Max, 10^3 Å	+11	+56	+1	+5	+18	+4
Min, 10^3 Å	-20	-9	-76	-73	-133	-73

Table S3. Molecular orbital (MO) energy levels in the B_{80} and $X@B_{80}$ complexes. Localization of MO is designated by capital letters: "(B)" – localized on B_{80}; "M" – localized on gas molecule; "D" – delocalized, i.e. shared by B_{80} and gas molecule.

Molecular Orbital	Energy of MO, eV						
	B_{80}	$CO_2@B_{80}$	$H_2@B_{80}$	$H_2S@B_{80}$	$HF@B_{80}$	$NH_3@B_{80}$	$SO_2@B_{80}$
LUMO+6	-3.4205	(B) -3.3666	(B) -3.3625	(B) -3.4308	(D) -3.4589	(B) -3.0580	(B) -3.5155
LUMO+5	-3.5623	(B) -3.6107	(B) -3.6113	(B) -3.6741	(B) -3.6806	(D) -3.1906	(B) -3.5209
LUMO+4	-3.5737	(B) -3.6115	(B) -3.6121	(B) -3.6768	(B) -3.6885	(B) -3.2790	(B) -3.5277
LUMO+3	-3.5835	(B) -3.6181	(B) -3.6134	(B) -3.6817	(D) -3.7087	(B) -3.3100	(B) -4.0064
LUMO+2	-4.0728	(B) -4.1011	(B) -4.1019	(B) -4.1645	(B) -4.1626	(D) -3.6727	(B) -4.0124
LUMO+1	-4.0826	(B) -4.1032	(B) -4.1024	(B) -4.1672	(B) -4.1764	(B) -3.7963	(B) -4.0183
LUMO	-4.0883	(B) -4.1076	(B) -4.1043	(B) -4.1734	(D) -4.2126	(B) -3.8050	(M) -4.5729
HOMO	-5.2031	(B) -5.2053	(B) -5.2159	(B) -5.2758	(B) -5.2665	(D) -4.6254	(B) -5.1003
HOMO-1	-5.2097	(B) -5.2069	(B) -5.2167	(B) -5.2782	(B) -5.2761	(B) -4.8981	(B) -5.1280
HOMO-2	-5.2167	(B) -5.2241	(B) -5.2184	(B) -5.2826	(B) -5.3008	(B) -4.9242	(B) -5.1340
HOMO-3	-5.2287	(B) -5.2320	(B) -5.2230	(B) -5.2883	(B) -5.3087	(B) -4.9348	(B) -5.1555
HOMO-4	-5.2369	(B) -5.2407	(B) -5.2238	(B) -5.2989	(B) -5.3237	(B) -4.9550	(B) -5.1571
HOMO-5	-5.9558	(B) -5.9664	(B) -5.9702	(M) -5.9332	(D) -6.0323	(D) -5.4483	(B) -5.8597
HOMO-6	-5.9583	(B) -5.9680	(B) -5.9713	(B) -6.0320	(B) -6.0372	(B) -5.6690	(B) -5.8782

Table S4. Electronic transitions predicted for B_{80} in vacuum and $X@B_{80}$ complexes. Transitions with oscillator strength (f) smaller than 0.001 are omitted.

#	Energy, eV	λ, nm	$f\times10^4$	Primary MO transitions HOMO→LUMO+M
B_{80}	1.7037	728	11	H-2→L+5 & H-3→L+6
	1.7064	727	45	H-3→L+5 & H-1→L+6
	1.7123	724	38	H-4→L+5
	1.7205	721	28	H-4→L+6
$CO_2@B_{80}$	1.6733	741	48	H-3→L+3 & H-2→L+4
	1.6761	740	52	H-4→L+3 & H-2→L+5
	1.6835	737	34	H-4→L+4
$H_2@B_{80}$	1.6702	742	57	H-2→L+5 & H→L+5
	1.6709	742	58	H-2→L+4 & H-3→L+5
	1.6714	742	56	H-3→L+4 & H-3→L+6
$H_2S@B_{80}$	1.6593	747	14	H-4→L+5 & H-1→L+3
	1.6683	743	53	H-3→L+3
	1.6728	741	54	H-4→L+3
	1.6770	739	40	H-4→L+4
	1.7698	701	10	H-5→L+1
	1.7723	700	21	H-5→L+2
$HF@B_{80}$	1.6601	767	22	H-3→L+4
	1.6666	744	36	H-3→L+5
	1.6755	740	48	H-2→L+5
	1.6921	733	24	H-4→L+5
$NH_3@B_{80}$	1.4003	885	39	H→L+4
	1.6715	742	18	H→L+8
	1.6945	732	32	H-4→L+3 & H-4→L+4
	1.7055	727	44	H-5→L+1
	1.7175	722	35	H-4→L+4
	1.7677	701	24	H-2→L+5
	1.7862	694	13	H-3→L+5
	1.8491	671	48	H-5→L+2
	1.8645	644	17	H-4→L+7
	1.9279	643	23	H-6→L
$SO_2@B_{80}$	1.3567	914	127	H-7→L
	1.6829	737	51	H-4→L+4
	1.6850	736	45	H-4→L+5
	1.6916	733	33	H-3→L+6

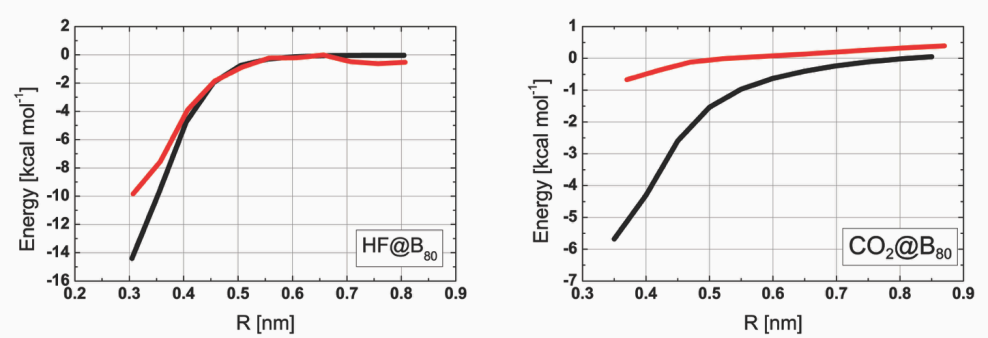

Figure S1: Binding energy versus intermolecular distance for the HF@B_{80} and CO_2@B_{80} complexes. Black and red stands for the curves with and without dispersion correction.

Whereas the dispersion correction (black curve) is essential for the proper description of the interaction energy between the counterparts of the complex, the electrostatic component (red curve) is significant and depends crucially on the dipole moment of the gas molecule.