Supporting data

Exploring adsorption behavior of O-contained VOCs in human breath on B_2N monolayer using DFT simulations

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Optimised geometries of the studied complexes

Acetone/B_2N:

		x	y	z
H	1	-0.00613	0.00345	0.00405
H	2	-0.00621	-0.00577	0.00039
H	3	-0.01672	0.00572	0.00549
H	4	-0.00023	0.02153	-0.00038
H	5	-0.00832	0.00027	0.00429
H	6	-0.01444	-0.00035	-0.00103
B	1	-0.00877	-0.00110	0.01532
B	2	-0.00550	-0.01927	0.00424
B	3	0.00104	-0.02240	0.01550
B	4	-0.01948	0.00262	0.01499
B	5	0.00114	-0.01248	0.00706
B	6	-0.00411	0.01279	0.00514
B	7	0.00826	0.00349	0.00113
B	8	-0.01334	-0.01827	-0.00193
B	9	0.00846	0.00385	-0.01525
B	10	-0.00302	-0.00282	-0.01288

B	11	0.01715	-0.00446	-0.00515
B	12	-0.00604	-0.00149	-0.01802
B	13	-0.01064	0.01186	-0.02407
B	14	0.00281	-0.01386	-0.01110
B	15	-0.00736	0.00691	0.01221
B	16	-0.00204	-0.00880	-0.00502
C	1	-0.00345	0.01778	-0.00419
C	2	0.01243	0.01682	0.01838
C	3	0.00892	0.01602	0.01146
N	1	0.02119	0.00847	0.00571
N	2	0.00387	-0.00001	0.00958
N	3	-0.00495	-0.01171	0.00532
N	4	0.01582	-0.01641	-0.01023
N	5	0.00610	-0.00622	-0.00386
N	6	-0.00560	0.01285	-0.01154
N	7	0.01614	-0.00607	-0.00134
N	8	0.00359	0.00556	-0.00603
O	1	0.01944	0.00151	-0.00824

Ethanol/B_2N:

		x	y	z
H	1	-0.00185	-0.01949	0.00368
H	2	0.03310	-0.01024	0.00610
H	3	0.00479	-0.00202	-0.02201
H	4	0.00196	-0.02718	0.01219
H	5	-0.01636	0.00228	-0.00971
H	6	0.01134	-0.00181	-0.00895
B	1	0.00199	0.00746	-0.00402
B	2	0.01372	0.01470	0.01028
B	3	-0.01063	0.01469	-0.01892

B	4	0.01847	0.01002	-0.00325
B	5	-0.00963	-0.01018	0.00247
B	6	0.02540	0.00300	-0.00096
B	7	0.01097	-0.00658	0.00068
B	8	0.00349	-0.01314	-0.00358
B	9	-0.00987	0.00876	-0.02030
B	10	0.00868	0.00793	0.00027
B	11	-0.00897	0.00834	0.00894
B	12	-0.03154	0.01657	-0.00448
B	13	-0.00301	0.00945	0.00249
B	14	0.00549	0.00293	0.00367
B	15	-0.02929	0.00369	-0.00336
B	16	-0.00842	-0.02860	0.00253
C	1	0.00326	0.00313	0.00050
C	2	-0.00256	-0.00122	0.00746
N	1	0.00923	0.01183	-0.00012
N	2	-0.02030	-0.00614	0.00650
N	3	0.00069	0.00257	-0.00619
N	4	-0.01959	-0.00521	0.02338
N	5	0.00309	0.00656	0.00966
N	6	-0.00497	0.00323	-0.01404
N	7	-0.00320	-0.00948	-0.01211
N	8	0.00803	0.00133	0.00543
O	1	0.01649	0.00282	0.02575

Methanol/B_2N:

		x	**y**	**z**
H	1	-0.01033	-0.01435	0.00188
H	2	0.02495	-0.01703	0.00103
H	3	0.00324	-0.00610	0.01893

H	4	-0.00831	-0.00454	-0.00490
B	1	0.01325	0.00413	-0.00845
B	2	0.00055	0.00412	-0.00256
B	3	0.01334	0.00513	0.00558
B	4	-0.01447	-0.00543	0.01143
B	5	-0.01969	-0.01297	0.00791
B	6	-0.01388	-0.00130	-0.00887
B	7	0.01256	-0.00623	0.00770
B	8	-0.02148	-0.00625	-0.01610
B	9	0.00097	0.00639	0.00376
B	10	0.00497	0.00111	0.01658
B	11	0.00466	0.01035	-0.01326
B	12	-0.00031	0.01363	0.02013
B	13	0.01043	0.00184	0.00994
B	14	-0.00301	0.00109	-0.02000
B	15	-0.00145	-0.00172	0.00233
B	16	0.00091	0.00695	-0.00650
C	1	-0.00924	-0.02059	-0.00292
N	1	0.01074	0.00613	-0.02618
N	2	0.01516	0.00140	-0.01935
N	3	-0.00088	0.00208	0.00097
N	4	-0.00971	0.00705	0.00371
N	5	-0.00306	0.01852	0.02736
N	6	0.01779	-0.00199	0.01201
N	7	-0.01571	-0.01584	-0.02770
N	8	0.00039	0.00708	0.00301
O	1	-0.00239	0.01732	0.00252

Formaldehyde/B_2N:

		x	y	z
H	1	-0.01330	0.00267	-0.00273
H	2	-0.01127	0.01197	-0.00475
B	1	-0.00310	-0.00507	0.02524
B	2	0.01240	-0.00645	-0.01134
B	3	0.01007	-0.00178	-0.02290
B	4	0.01359	0.01793	0.00252
B	5	-0.00047	0.00109	-0.00844
B	6	0.00272	0.01075	-0.00300
B	7	0.00660	-0.01274	-0.01026
B	8	0.00035	-0.01535	-0.00331
B	9	0.00739	0.00486	-0.00028
B	10	-0.00367	-0.01839	0.02046
B	11	0.00268	-0.00080	0.00144
B	12	-0.01311	-0.00582	0.00503
B	13	-0.01713	-0.00551	0.00534
B	14	0.00551	-0.02818	-0.00336
B	15	-0.00867	-0.00152	0.00387
B	16	-0.00216	0.00474	0.00256
C	1	0.00119	0.01657	0.01224
N	1	0.00292	-0.00456	-0.00907
N	2	0.00930	0.00085	-0.00403
N	3	0.01345	-0.00944	-0.00479
N	4	0.00510	-0.00639	-0.01495
N	5	0.00011	0.00878	0.00400
N	6	0.00423	0.00639	0.00810
N	7	-0.00435	0.02195	0.00055
N	8	-0.00428	0.00448	0.00039
O	1	-0.01610	0.00895	0.01148