Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2018

Nitrogen Doped Nanohoops as Promising CO_2 Capturing Devices

Angel Vidal Vidal,[a] Carlos Silva López,[a] and Olalla Nieto Faza[b,*]

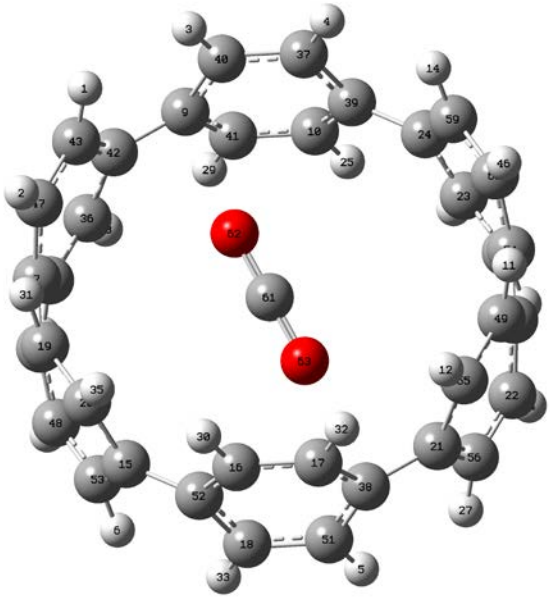
faza@uvigo.es

[a] Dpto. de Química Orgánica, Facultade de Química, Universidade de Vigo. Lagoas-Marcosende 36310, Vigo, Spain

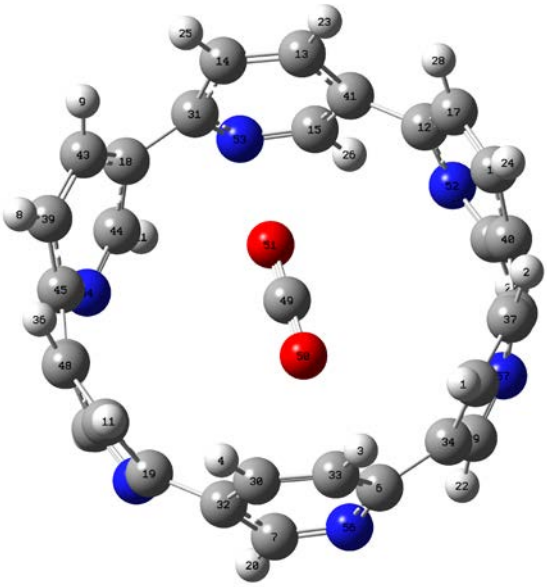
[b] Dpto. de Química Orgánica, Facultade de Ciencias, Universidade de Vigo. Campus As-Lagoas 32004, Ourense, Spain

Pages

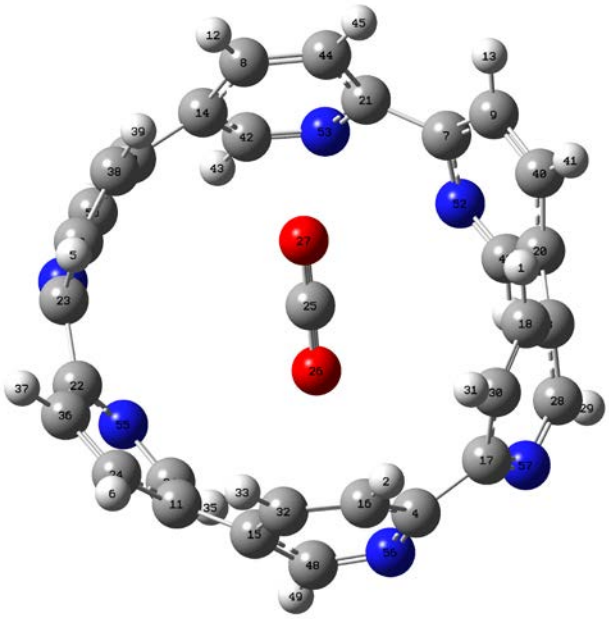
[6]-CPP



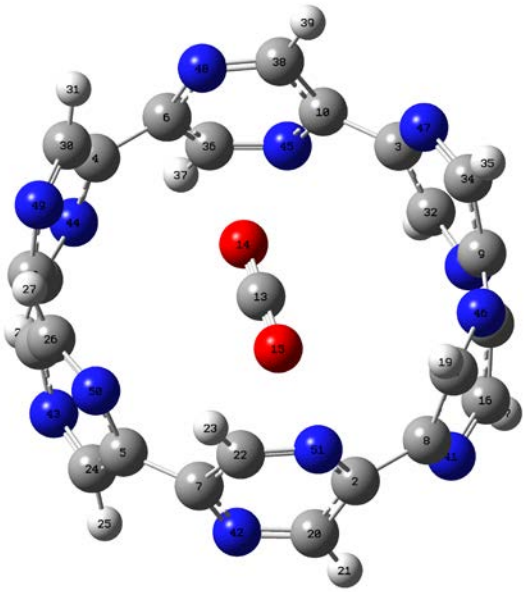
Aza-1a-[6]-CPP



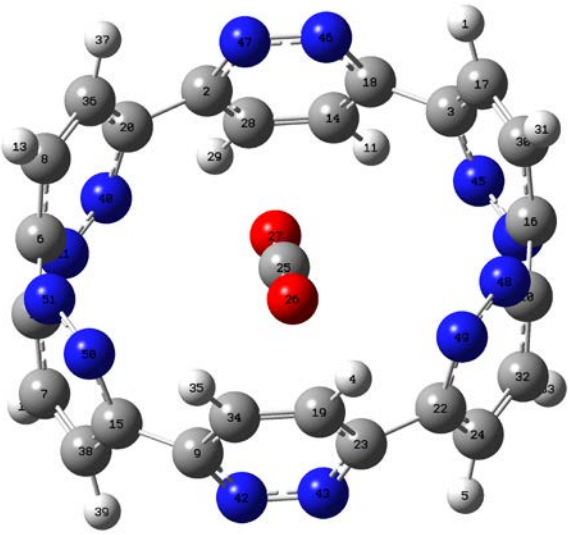
Aza-1b-[6]-CPP



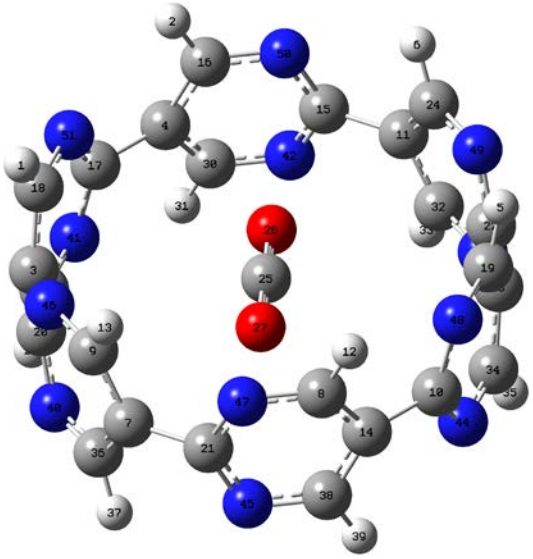
Aza-2a-[6]-CPP



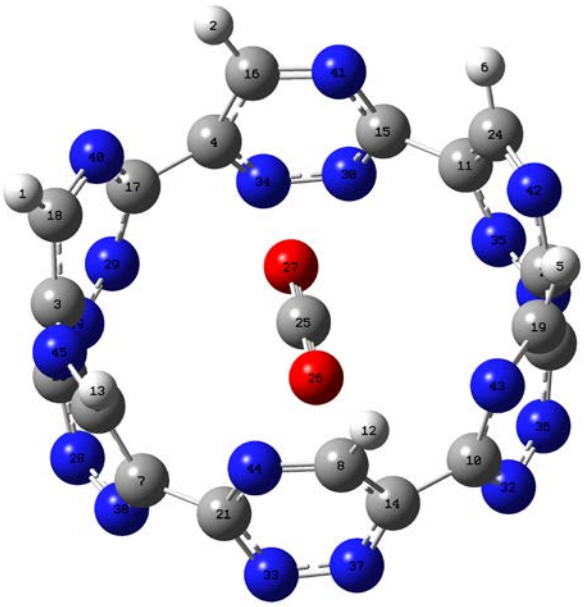
Aza-2b-[6]-CPP



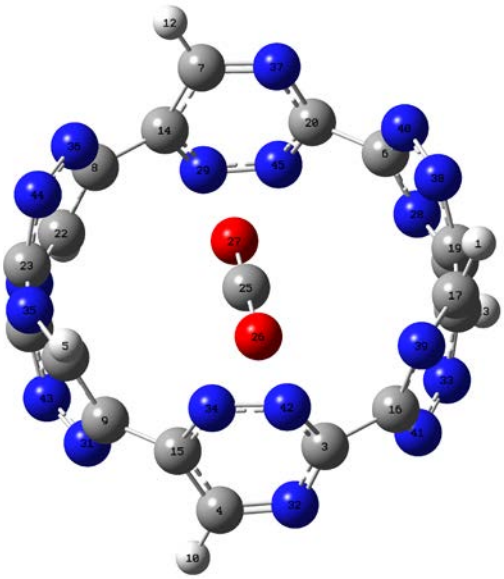
Aza-2c-[6]-CPP



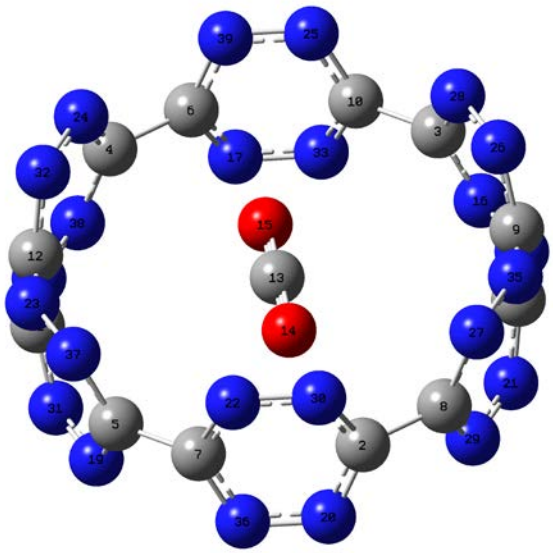
Aza-3a-[6]-CPP



Aza-3b-[6]-CPP



Aza-4a-[6]-CPP


39
25
24
6
10
28
4
3
26
17
33
32
16
15
30
9
12
13
35
23
14
27
37
21
31
5
22
38
8
2
29
19
7
36
20

SI2: Influence of free rotation of the guest on the final spectrum

To check the thermal variation of all the relevant IR signals in the complex, we simulated the effect of the conformational flexibility of carbon dioxide inside the nanohoop. Structures every 10 degrees of the rotation profile of carbon dioxide (in addition to the global minimum reported) were taken and we followed the procedure described in the Computational Methods section to compute the corresponding signals for all the bands reported on the manuscript.

Assuming an equal participation of all the species considered (a worst case scenario implying that all conformations are isoenergetic) the average value and the standard deviation for each band were computed.

Rotation angle (º)	vc^- (cm^{-1})	vc^+ (cm^{-1})	v_{2a} (cm^{-1})	v_{2b} (cm^{-1})	v_3 (cm^{-1})
6	1346,70	1456,07	689,49	692,77	2452,04
16	1348,03	1454,82	691,80	694,59	2445,09
26	1343,45	1452,53	688,03	691,25	2444,64
36	1343,99	1452,78	687,99	692,12	2445,24
46	1344,32	1453,92	687,30	692,36	2449,77
56	1345,83	1455,62	687,73	693,27	2451,70
66	1342,73	1454,20	683,75	692,76	2450,50
76	1344,08	1453,16	686,59	693,31	2448,12
minimum	1344,04	1454,94	682,20	696,09	2449,10

Average (cm-1)	1344,80	1454,23	687,84	692,80	2448,47
STD	1,70	1,24	2,86	1,43	2,87