

A comprehensive DFT study on sensing abilities of cyclic oligothiophenes

(nCT)

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Pakistan

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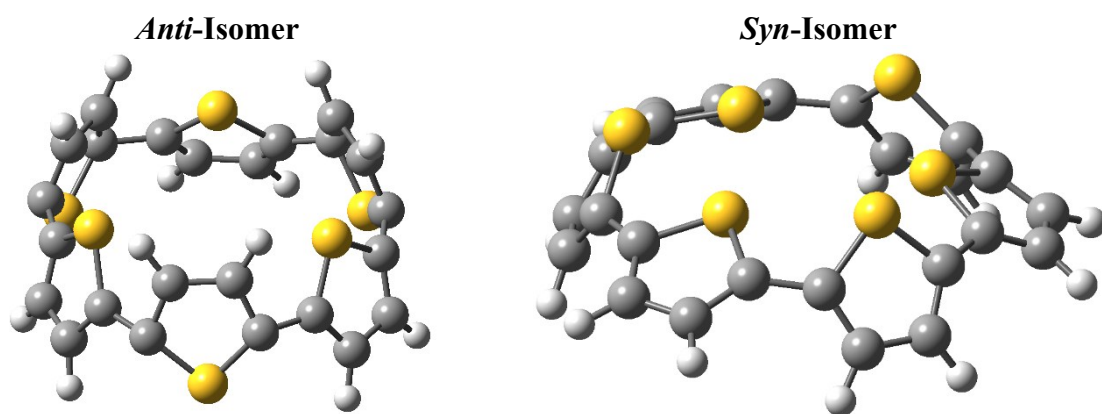
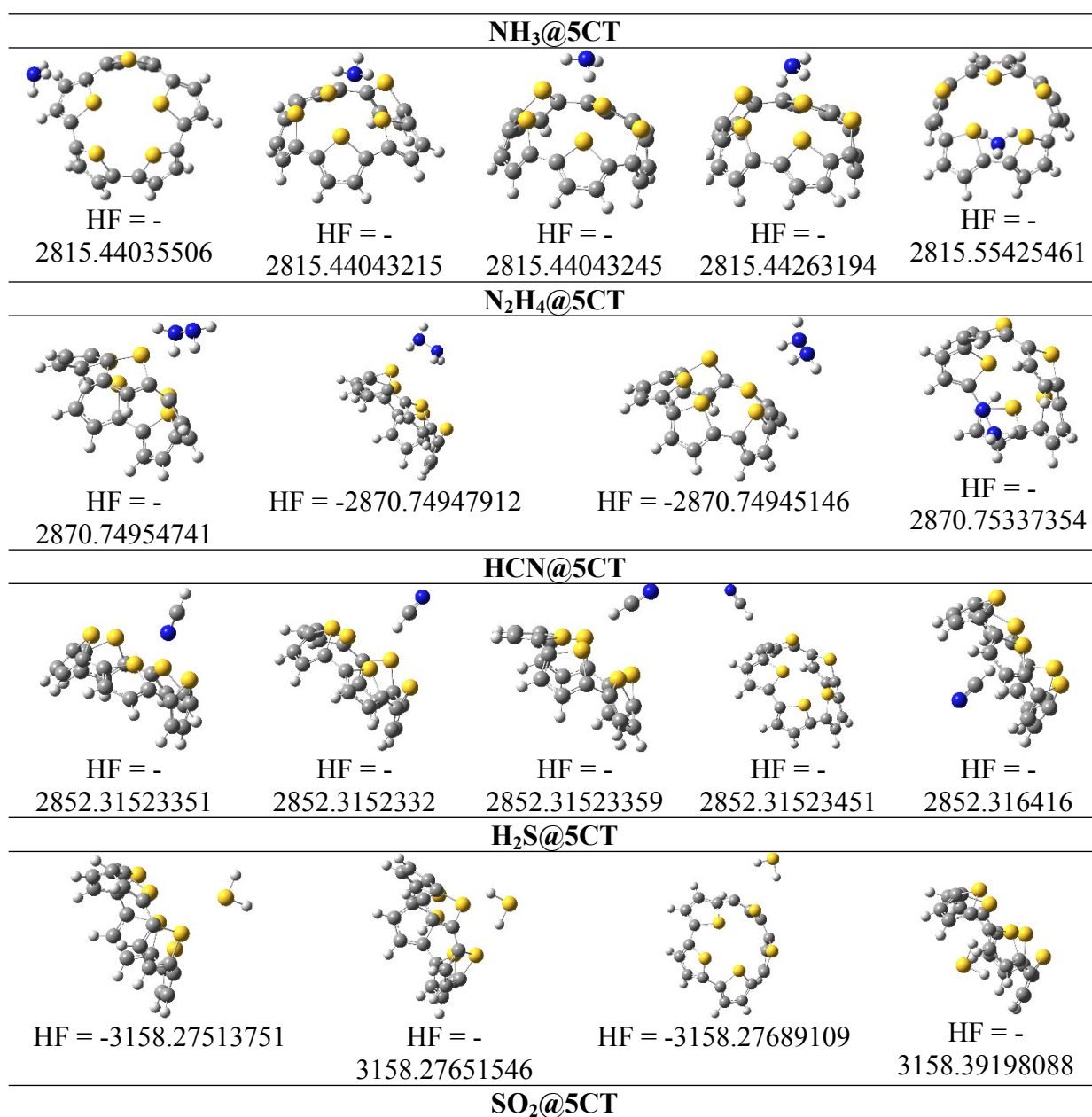
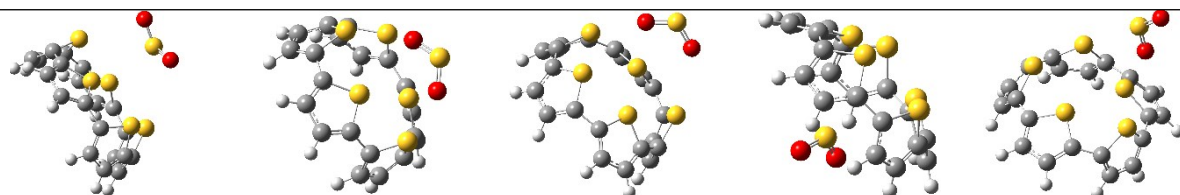


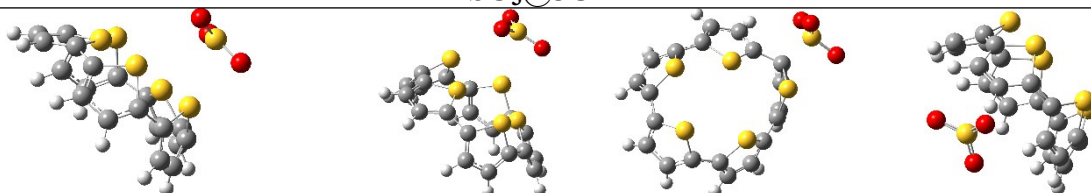
Figure S1a. Structures of anti- and syn-isomers of cyclic oligothiophene.





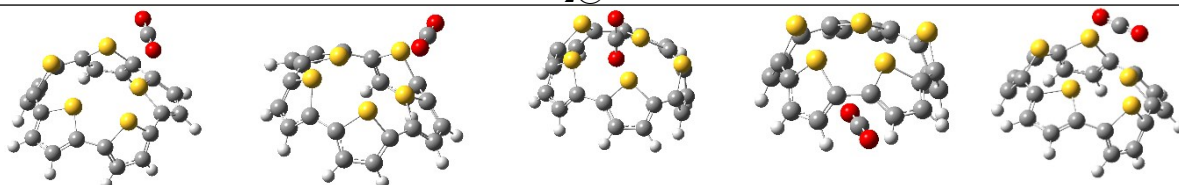
HF = -
3307.47996333 HF = -
3307.47952844 HF = -
3307.47952844 HF = -
3307.4831405 HF = -
3307.48326389

SO₃@5CT



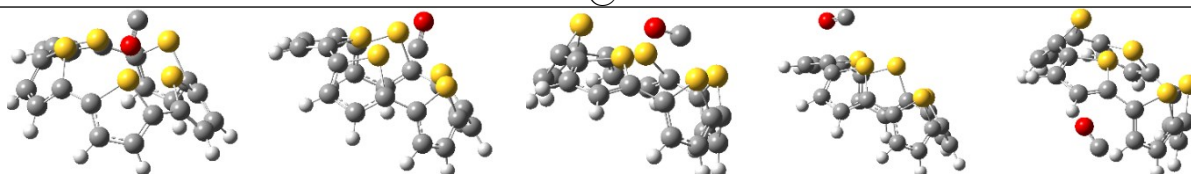
HF = -3382.65555663 HF = -
3382.65249989 HF = -
3382.68890325 HF = -
3382.66411207

CO₂@5CT



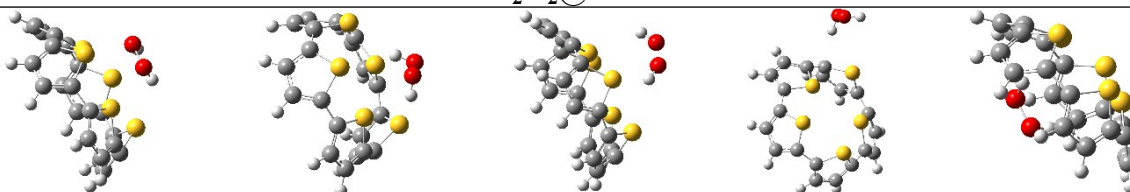
HF = -
2947.47236607 HF = -
2947.47236599 HF = -
2947.47193746 HF = -
2947.47302084 HF = HF = -
2947.47192

CO@5CT



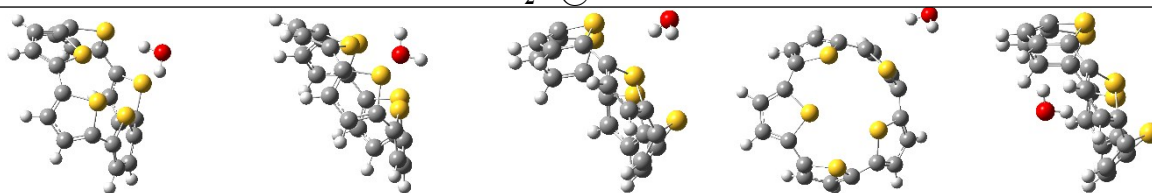
HF = -
2872.20002584 HF = -
2872.20005746 HF = -
2872.20003480 HF = -
2872.19995561 HF = -
2872.200507

H₂O₂@5CT



HF = -
2910.42930128 HF = -
2910.42930178 HF = -
2910.429096 HF = -
2910.4286791 HF = -
2910.54934016

H₂O@5CT



HF = -
2835.30414092 HF = -
2835.30414092 HF = -
2835.30414088 HF = -
2835.30329189 HF = -
2835.3069489

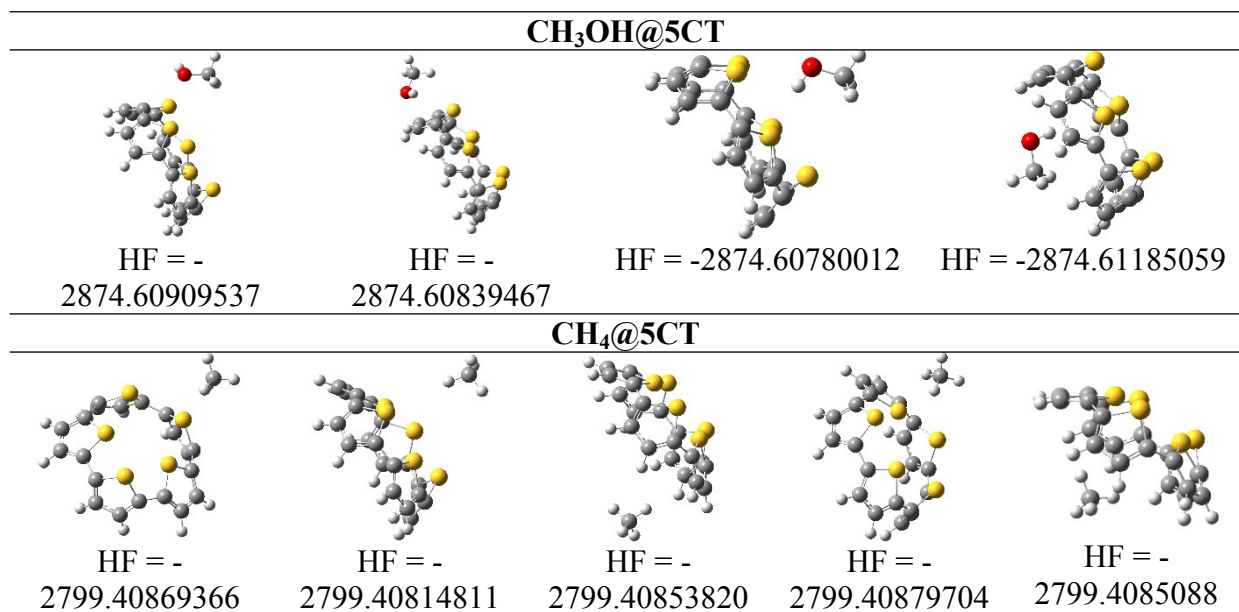
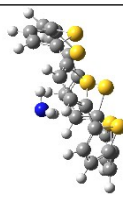
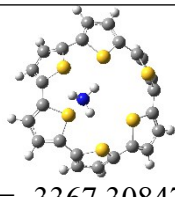


Figure S2a. Optimized geometries of analytes@5CT complexes

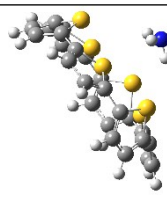
NH₃@6CT



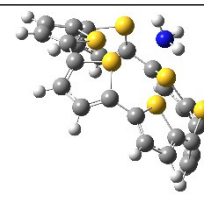
HF = -
3367.30838214



HF = -3367.30847200

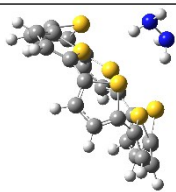


HF = -
3367.30689141

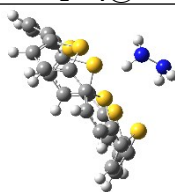


HF = -3367.30627441

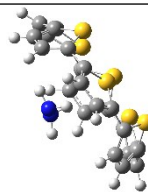
N₂H₄@6CT



HF = -3422.61579906

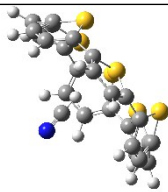


HF = -3422.61605595

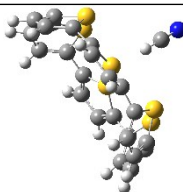


HF = -3422.61605582

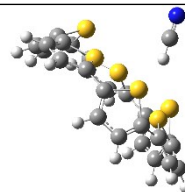
HCN@6CT



HF = -
3404.18400642



HF = -
3404.17729849

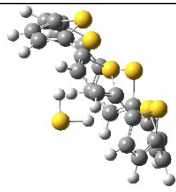


HF = -3404.18144858

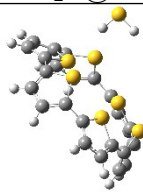


HF = -
3404.18252579

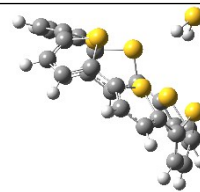
H₂S@6CT



HF = -3710.14408371

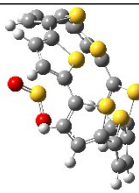


HF = -3710.14265945

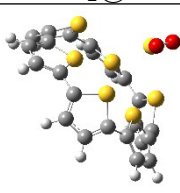


HF = -3710.14256426

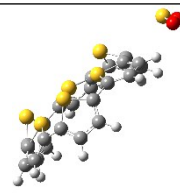
SO₂@6CT



HF = -3859.34869136

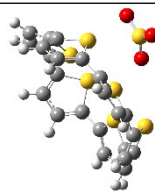


HF = -3859.34629632

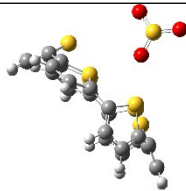


HF = -3859.34901495

SO₃@6CT



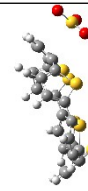
HF = -
3934.51866697



HF = -
3934.51587227



HF = -3934.52131815



HF = -3934.52350546

CO₂@6CT

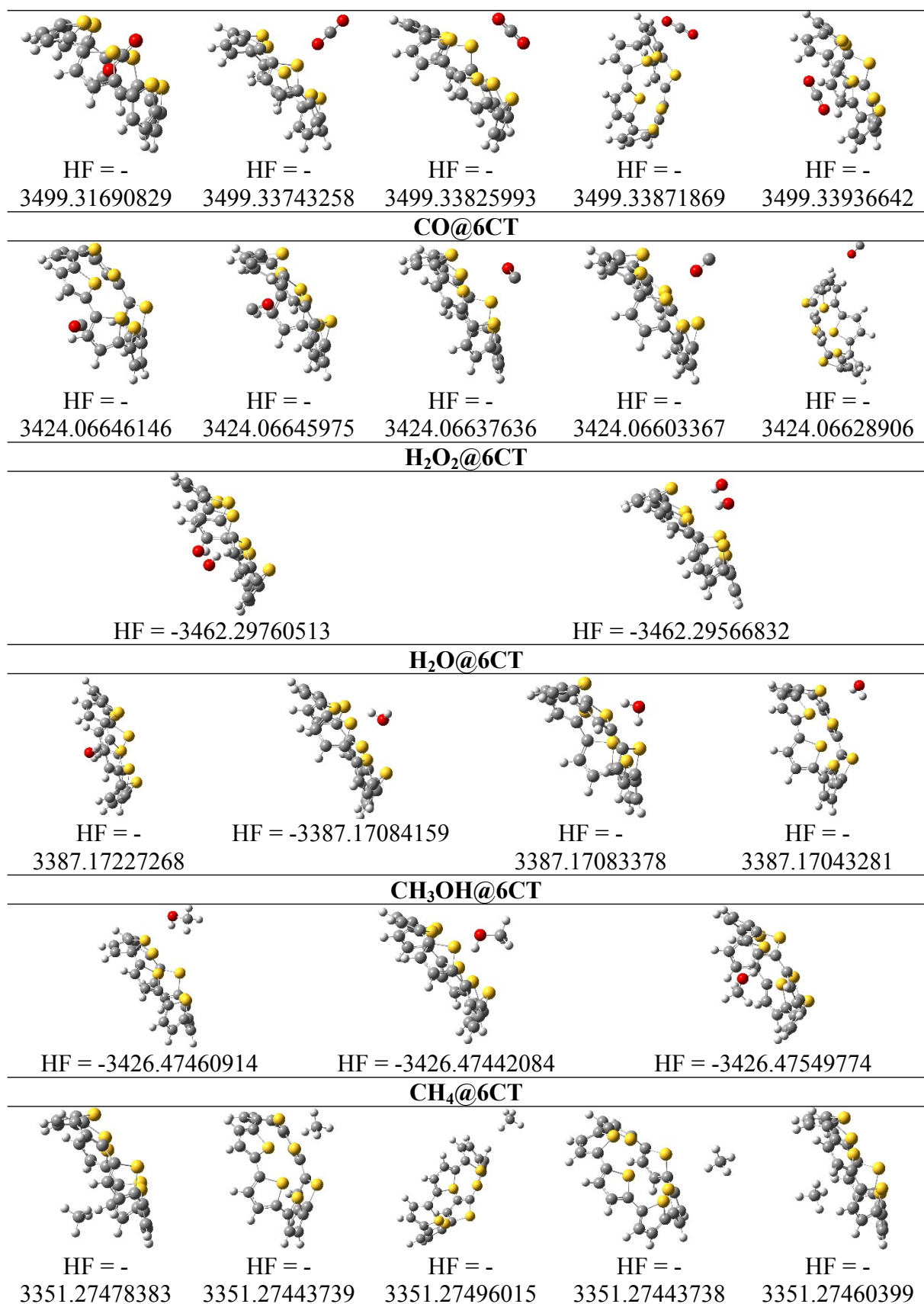
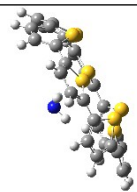
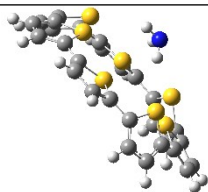


Figure S2b. Optimized geometries of analytes@6CT complexes

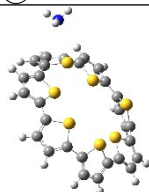
NH₃@7CT



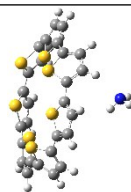
HF = -
3919.15789



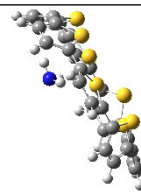
HF = -3919.1561899



HF = -
3919.1588129

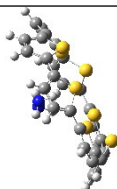


HF = -
3919.158545

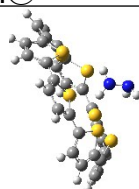


HF = -
3919.30088573

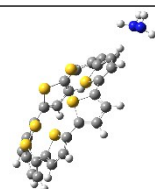
N₂H₄@7CT



HF = -3974.46863966

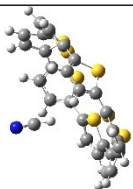


HF = -3974.46597895

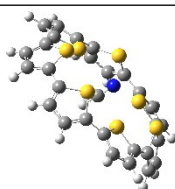


HF = -
3974.46641649

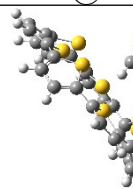
HCN@7CT



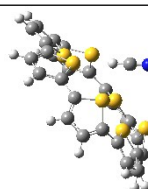
HF = -
3956.0322947



HF = -
3956.03081051



HF = -
3956.03081051



HF = -
3956.03081044

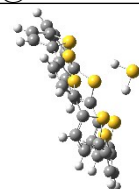


HF = -
3956.03155763

H₂S@7CT



HF = -3956.03155763

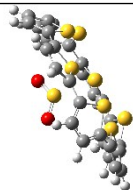


HF = -4261.99193257

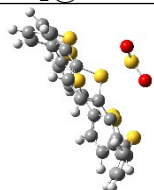


HF = -
4261.99236617

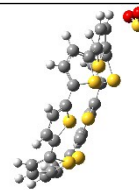
SO₂@7CT



HF = -4411.19697972

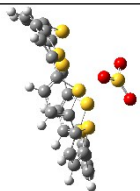


HF = -4411.19520905

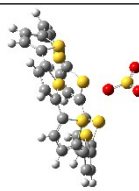


HF = -4411.19812346

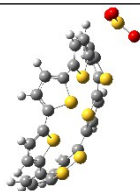
SO₃@7CT



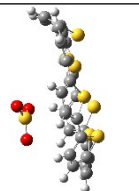
HF = -
4486.36783551



HF = -
4486.36783550

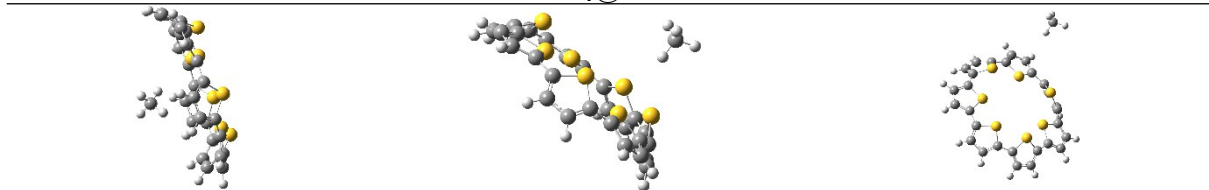
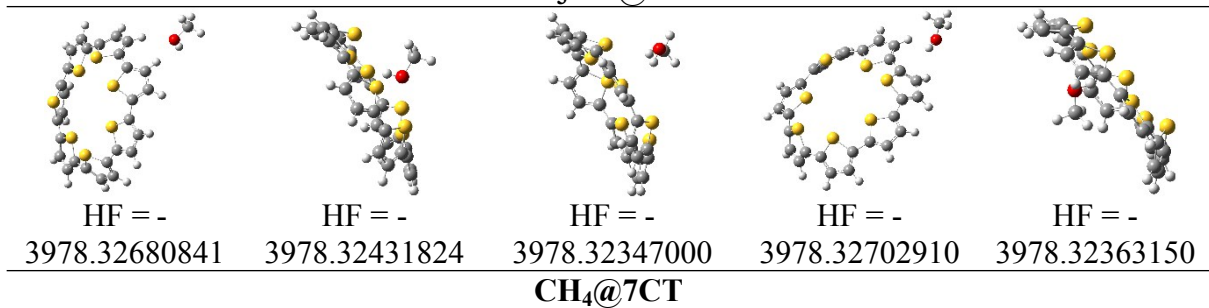
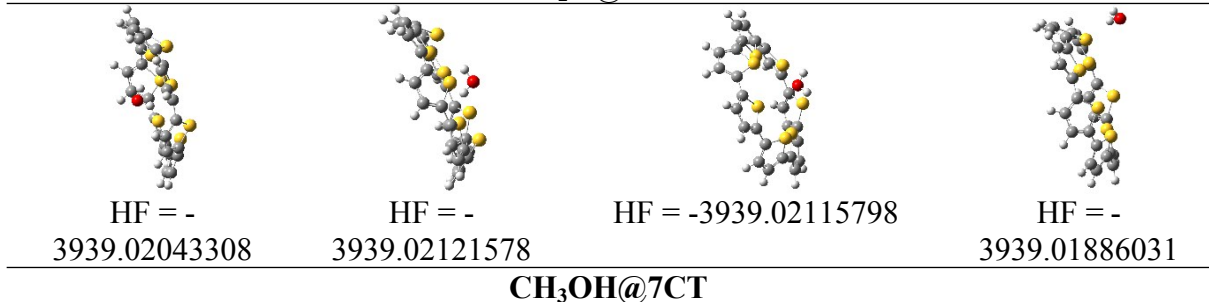
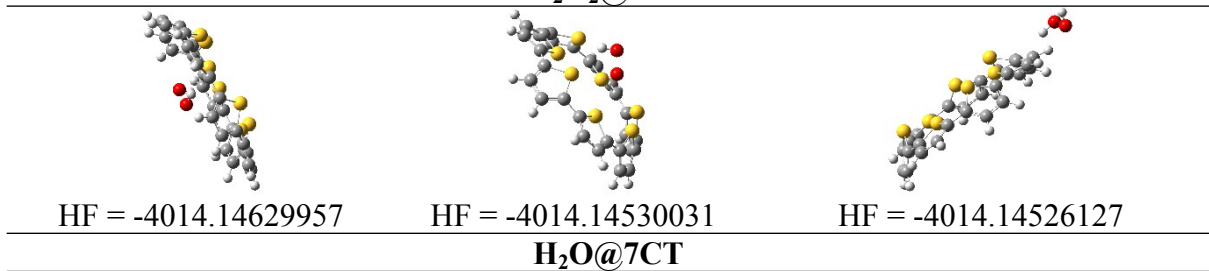
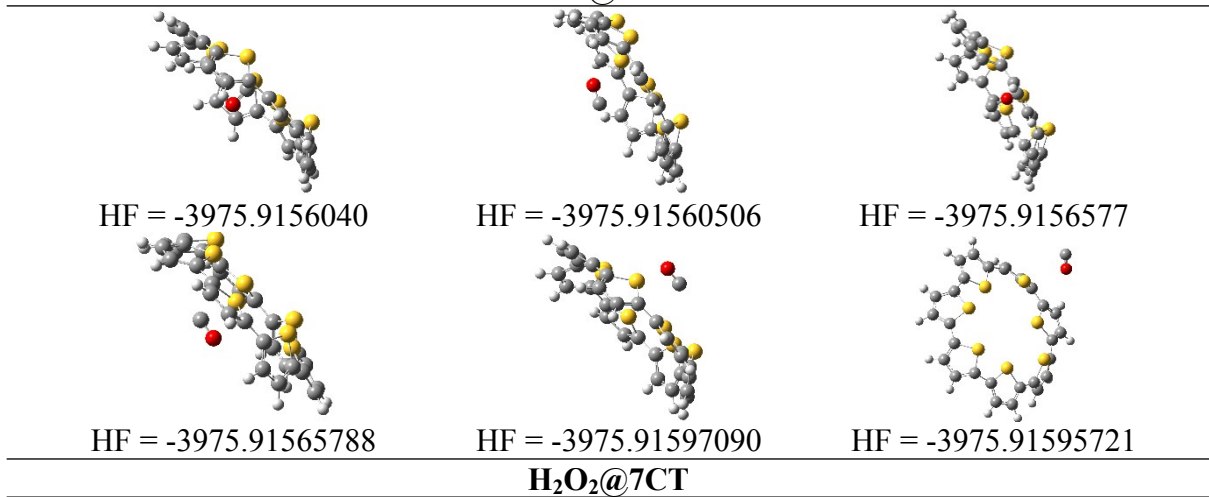
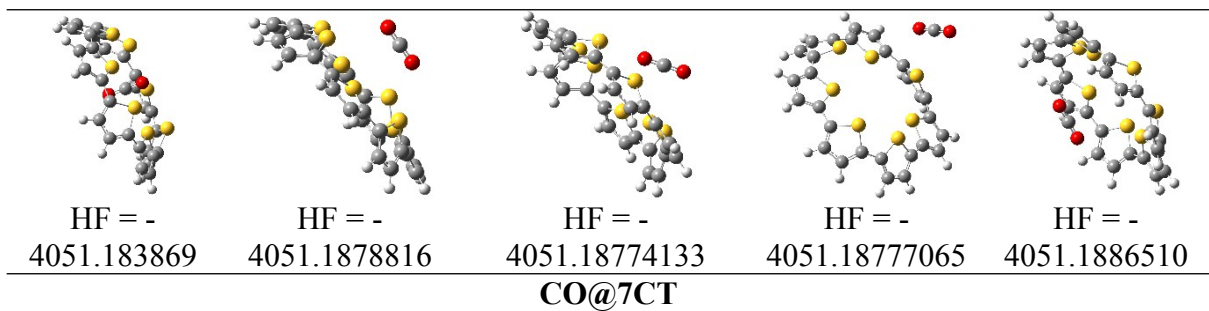


HF = -
4486.37446891



HF = -4486.37157432

CO₂@7CT



HF = -3903.12379933

HF = -3903.12374938

HF = -3903.12413762

Figure S2c. Optimized geometries of analytes@7CT complexes

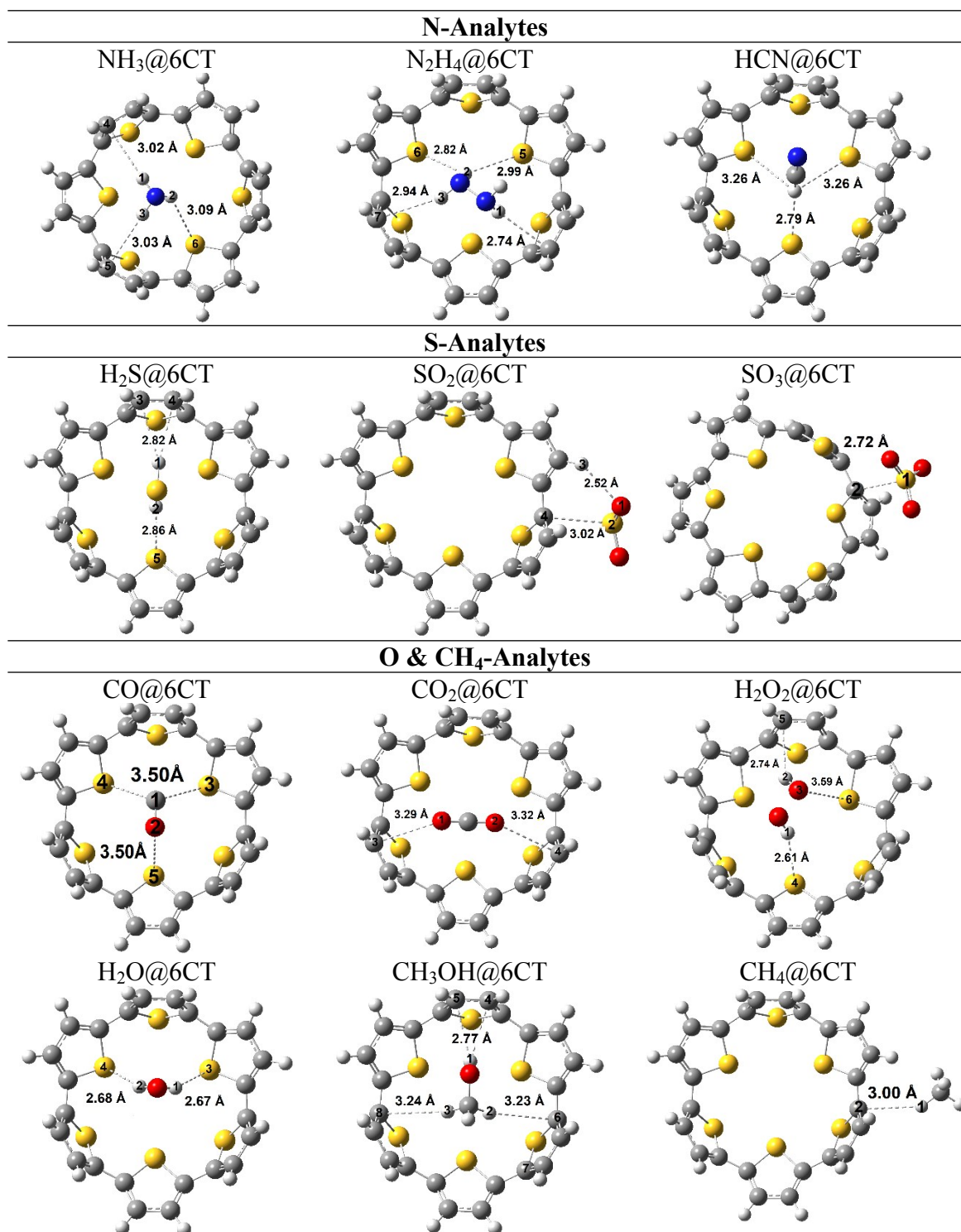


Figure S3a. The most stable geometries of analytes@6CT complexes. In grey: C; yellow: S; white: H; red: O and blue: N

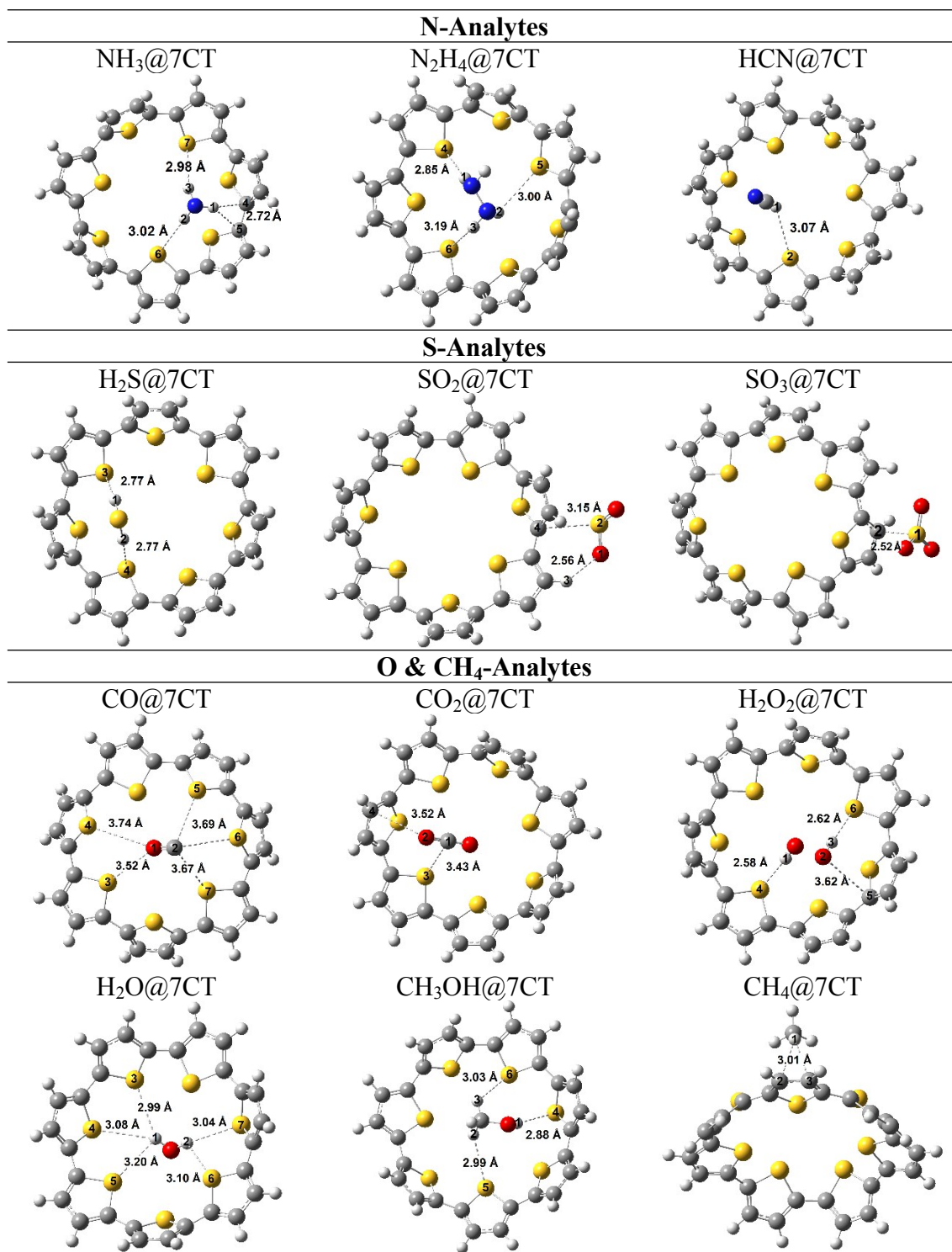
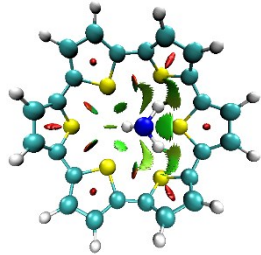
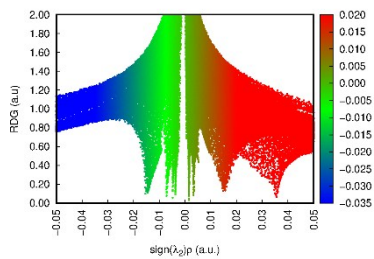


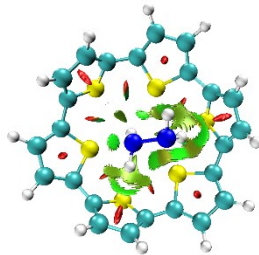
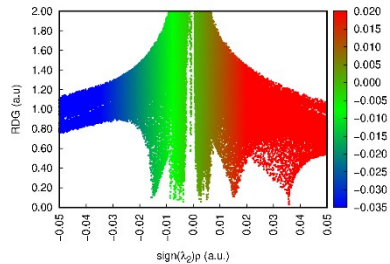
Figure S3b. The most stable geometries of analytes@7CT complexes. In grey: C; yellow: S; white: H; red: O and blue: N

N-Analytes

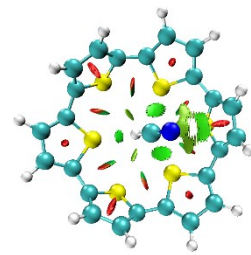
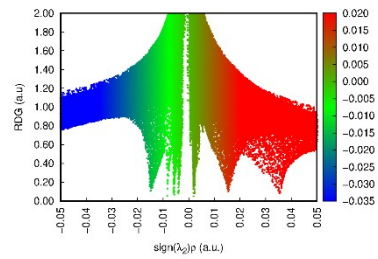
NH₃@6CT



N₂H₄@6CT

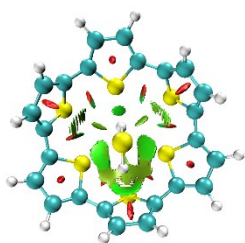
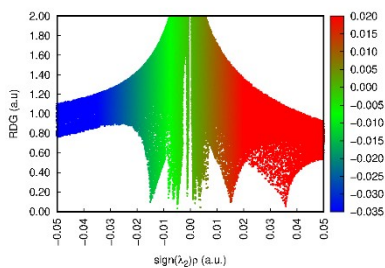


HCN@6CT

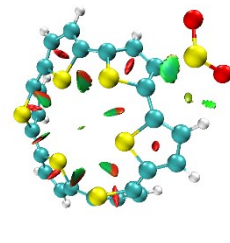
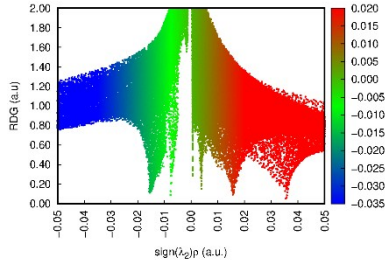


S-Analytes

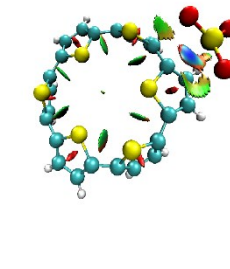
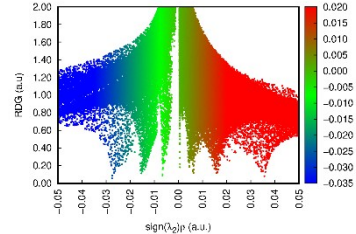
H₂S@6CT



SO₂@6CT

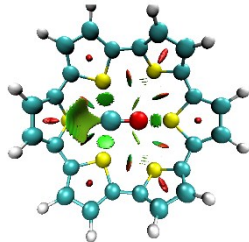
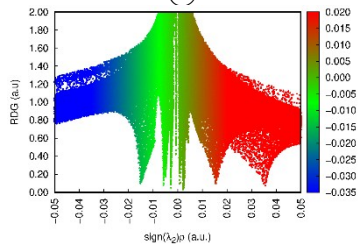


SO₃@6CT

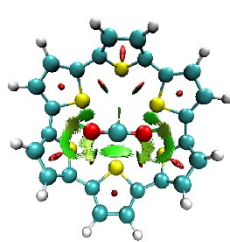
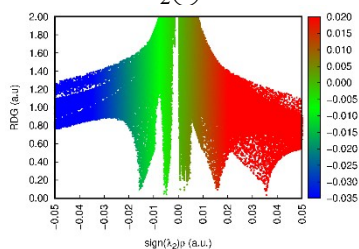


O & CH₄-Analytes

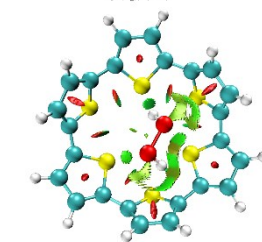
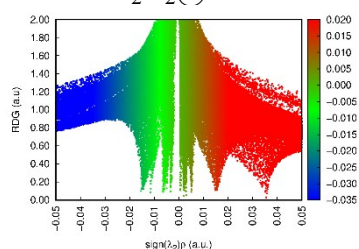
CO@6CT



CO₂@6CT



H₂O₂@6CT



H₂O@6CT

CH₃OH@6CT

CH₄@6CT

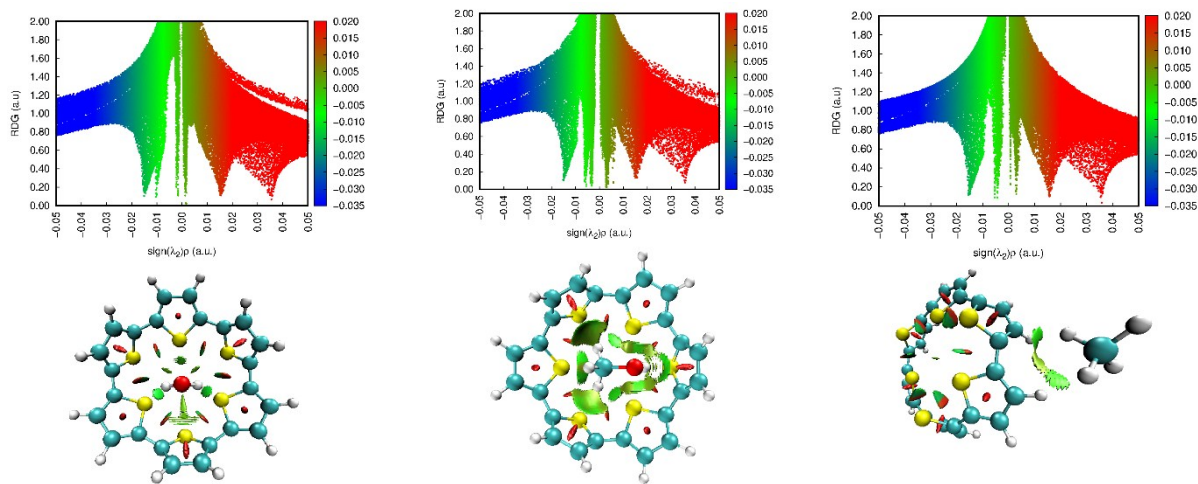


Figure S4a. NCI index with isovalue = 0.5 au and plot of reduced density gradient (RDG) versus $\text{sign}(\lambda_2)\rho(r)$ of analytes@6CT complexes.

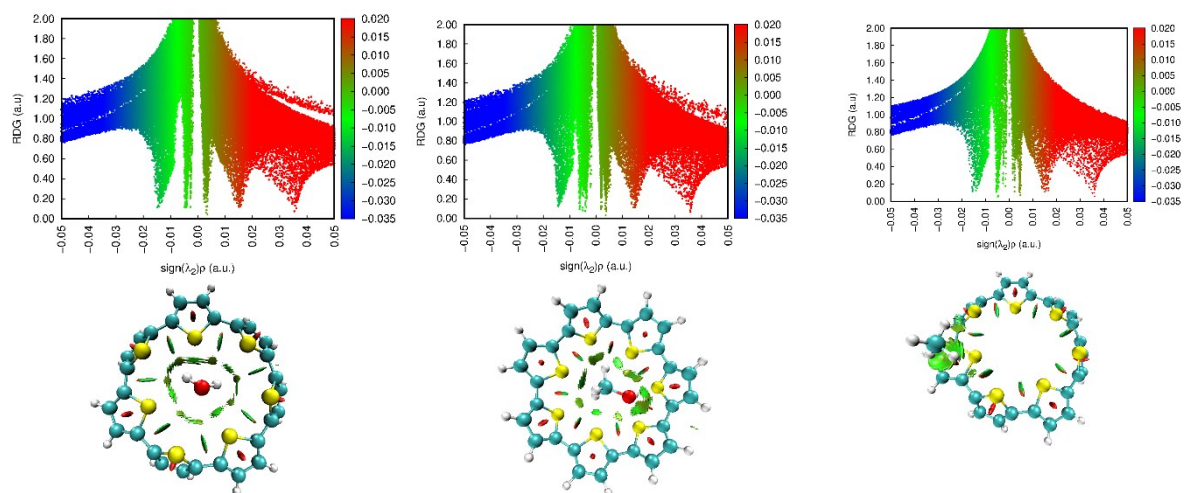
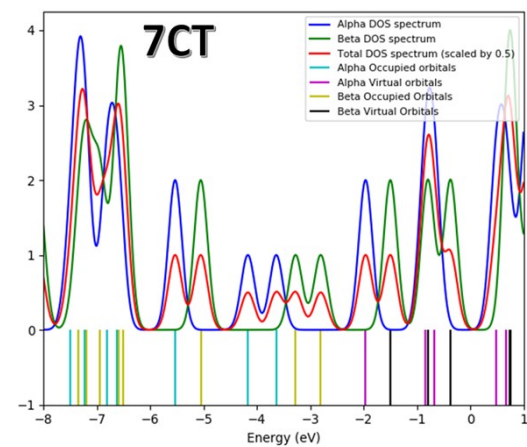
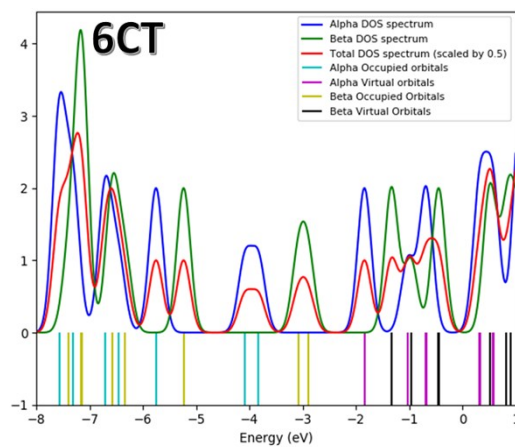
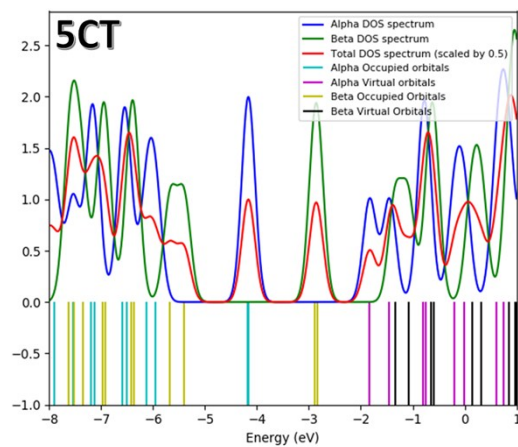
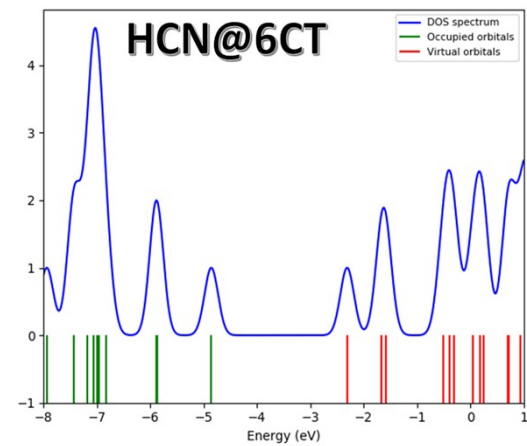
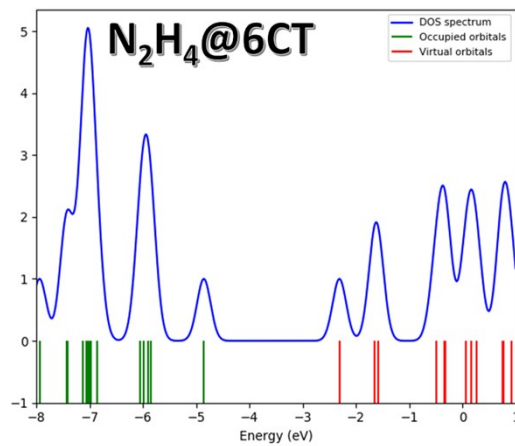
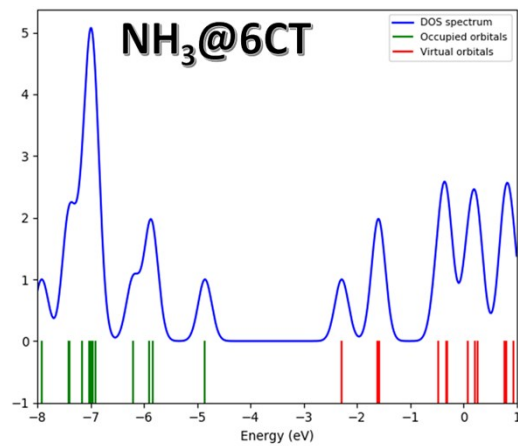


Figure S4b. NCI index with isovalue = 0.5 au and plot of reduced density gradient (RDG) versus $\text{sign}(\lambda_2)\rho(r)$ of analytes@7CT complexes.

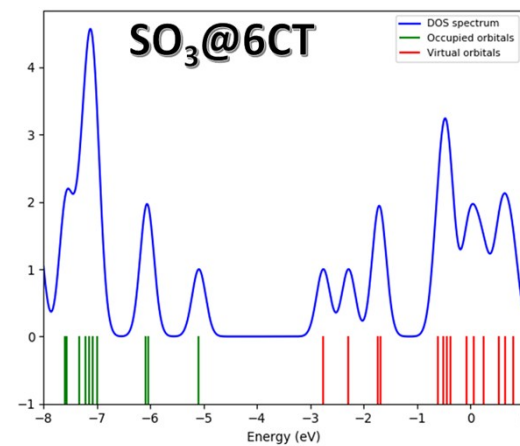
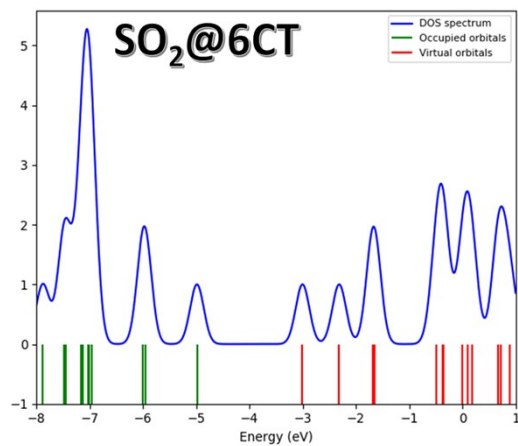
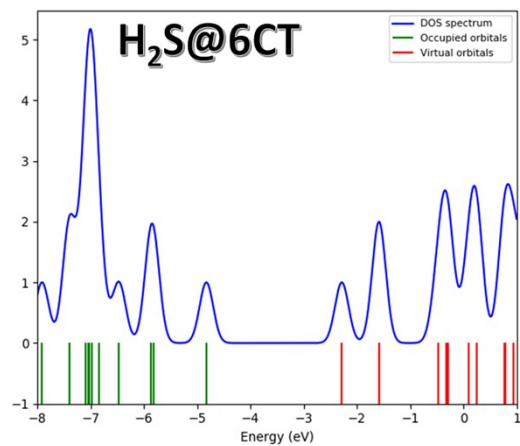
Pure nCT



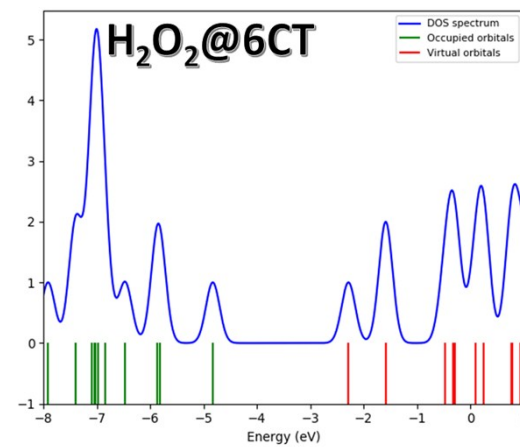
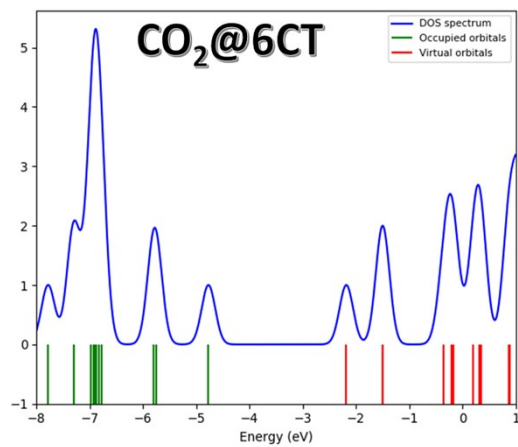
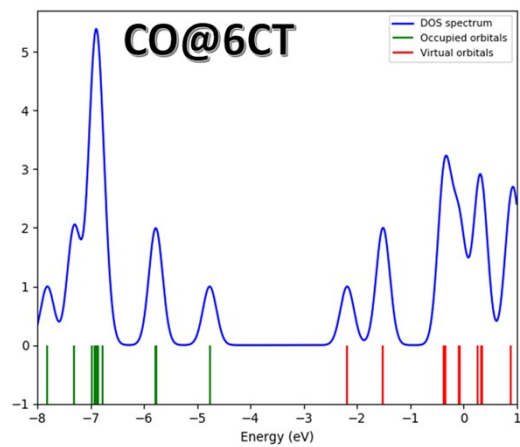
N-Analytes



S-Analytes



O & CH₄-Analytes



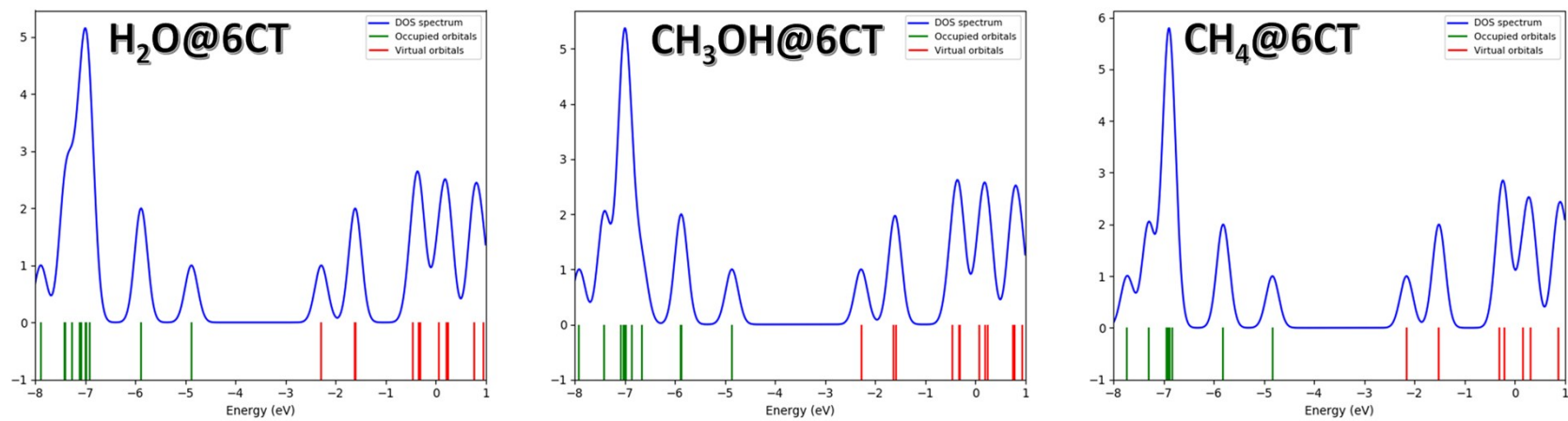
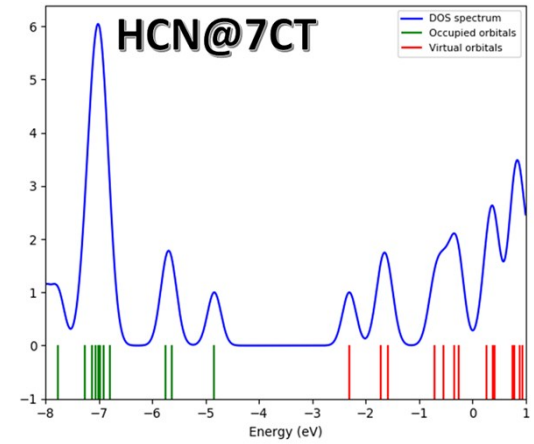
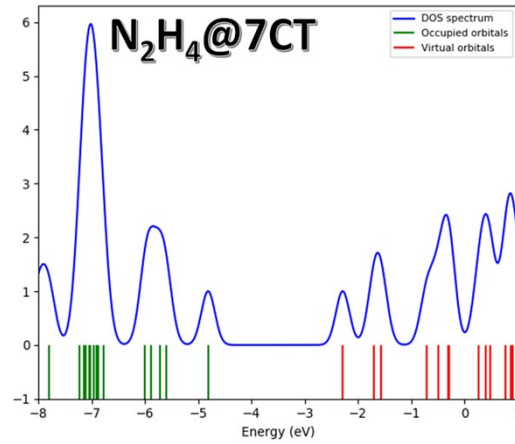
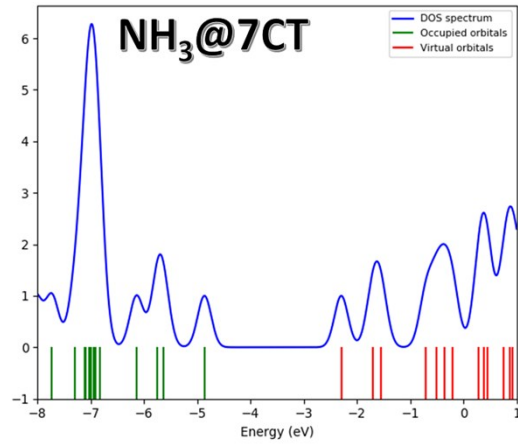
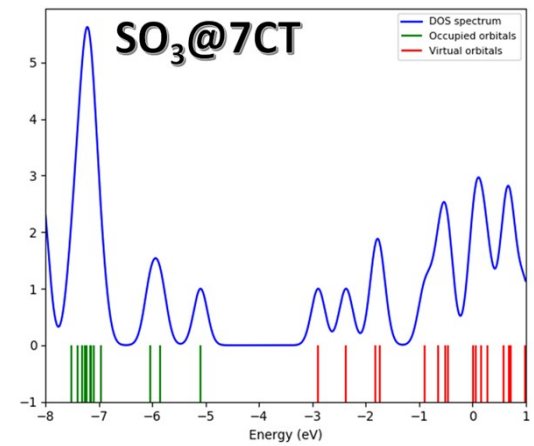
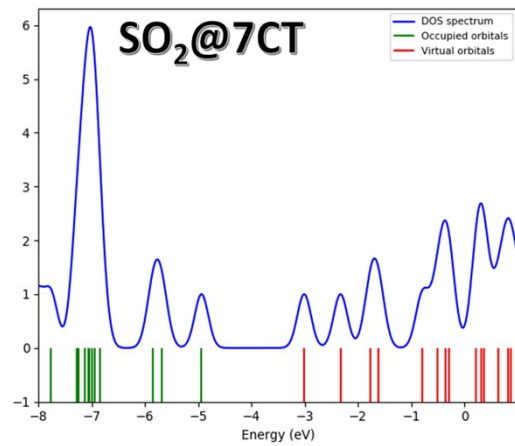
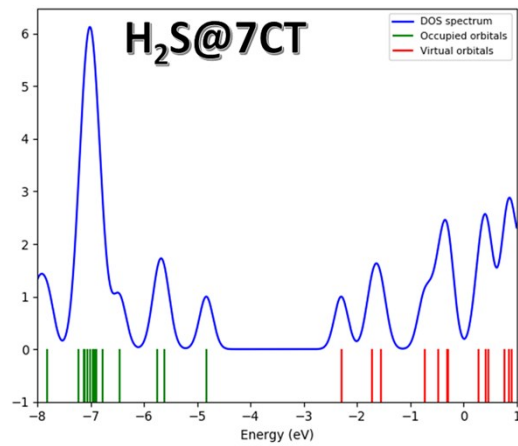


Figure S5a. DOS spectra of pure nCT and analytes@6CT complexes.

N-Analytes



S-Analytes



O & CH₄-Analytes

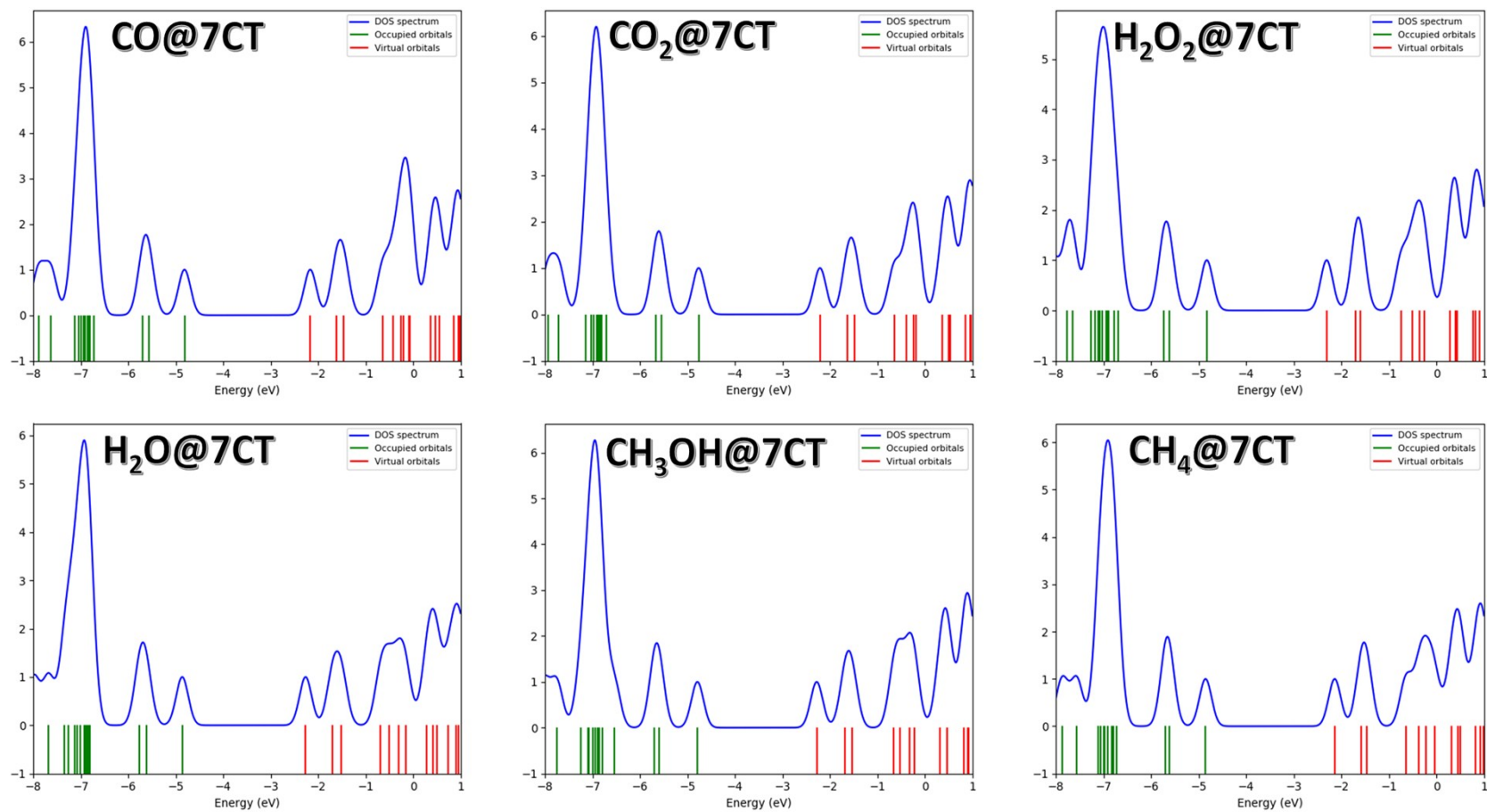


Figure S5b. DOS spectra of analytes@7CT complexes.

Table S1. Excited states and their transitions.

Complexes	Excited state	Major excitations	Complexes	Excited state	Major excitations
Pure nCT			CH₄-Analyte		
5CT	12	H-1→L+1 H→L	CH₄@5CT	6	H-1→L H→L+1
6CT	14	H-1→L H→L+1	CH₄@6CT	7	H-2→L H→L+2
7CT	12	H-1→L H-1→L+1 H→L, H→L+1	CH₄@7CT	8	H-1→L H→L+1
N-Analytes			S-Analytes		
NH₃@5CT	6	H-1→L H→L+1	H₂S@5CT	6	H-1→L H→L+1
NH₃@6CT	7	H-2→L H→L+2	H₂S@6CT	7	H-2→L H→L+1, H→L+2
NH₃@7CT	7	H-1→L H→L+1	H₂S@7CT	7	H-1→L H→L+1
N₂H₄@5CT	6	H-1→L H→L+1	SO₂@5CT	5	H-1→L H→L, H→L+2
N₂H₄@6CT	7	H-1→L H→L+1	SO₂@6CT	3	H→L H→L+1
N₂H₄@7CT	7	H-1→L H→L+1	SO₂@7CT	3	H→L
HCN@5CT	6	H-1→L H→L+1	SO₃@5CT	12	H-3→L H-2→L+1
HCN@6CT	6	H-1→L H→L+1	SO₃@6CT	6	H-2→L H→L, H→L+1
HCN@7CT	7	H-1→L H→L+1	SO₃@7CT	6	H-1→L H→L, H→L+1
O-Analytes					
CO@5CT	6	H-1→L H→L+1	H₂O₂@5CT	6	H-1→L H→L+1
CO@6CT	7	H-1→L H→L+2	H₂O₂@6CT	7	H-1→L H→L+2
CO@7CT	8	H-1→L H→L+1	H₂O₂@7CT	7	H-1→L H→L+1
CO₂@5CT	6	H-1→L H→L+1	H₂O@5CT	6	H-1→L H→L+1
CO₂@6CT	7	H-1→L H→L+2	H₂O@6CT	7	H-1→L H→L+1
CO₂@7CT	7	H-1→L H→L+1	H₂O@7CT	7	H-1→L H→L+1
CH₃OH@5CT	6	H-1→L H→L+1	CH₃OH@7CT	7	H-1→L H→L+1
T			T		
CH₃OH@6CT	7	H-1→L H→L+2			
T					

Table S2a. Molecular volume, molecular size and dipole moment of analyte@nCT complexes.

Species	Volume (cm ³ mol ⁻¹)	Sizes (Å)	Dipole (Debye)
N-Analytes			
NH ₃ @5CT	268.216	9.59	3.2940
NH ₃ @6CT	339.873	10.35	3.6315
NH ₃ @7CT	416.326	12.94	3.2483
N ₂ H ₄ @5CT	274.716	9.69	3.7381
N ₂ H ₄ @6CT	358.244	10.37	3.4757
N ₂ H ₄ @7CT	370.881	12.92	3.5397
HCN@5CT	259.062	9.62	2.2481
HCN@6CT	348.665	10.33	3.5638
HCN@7CT	403.569	12.92	3.3116
S-Analytes			
H ₂ S@5CT	294.923	9.62	3.7801
H ₂ S@6CT	328.065	10.29	4.1174
H ₂ S@7CT	375.843	12.94	3.7455
SO ₂ @5CT	295.406	9.70	7.2809
SO ₂ @6CT	394.953	10.48	5.2700
SO ₂ @7CT	314.977	12.99	5.2986
SO ₃ @5CT	304.345	8.96	19.6032
SO ₃ @6CT	337.219	10.42	8.6282
SO ₃ @7CT	369.713	13.01	8.1515
O-Analytes			
CO@5CT	255.457	9.62	4.8164
CO@6CT	382.382	10.398	5.1459
CO@7CT	416.513	13.00	4.8044
CO ₂ @5CT	290.847	9.68	4.7940
CO ₂ @6CT	268.465	10.42	5.2155
CO ₂ @7CT	406.927	12.97	5.0427
H ₂ O ₂ @5CT	273.056	9.67	3.1892
H ₂ O ₂ @6CT	364.082	10.32	3.2242
H ₂ O ₂ @7CT	459.124	12.899	3.3459
H ₂ O@5CT	281.19	9.66	3.3800
H ₂ O@6CT	325.455	10.38	3.3765
H ₂ O@7CT	357.102	13.02	6.4734
CH ₃ OH@5CT	312.762	9.59	3.2136
CH ₃ OH@6CT	285.474	10.35	3.6679
CH ₃ OH@7CT	372.592	12.91	4.1316
CH₄-Analytes			
CH ₄ @5CT	322.43	9.71	4.8514
CH ₄ @6CT	326.62	10.46	4.9313
CH ₄ @7CT	436.47	13.03	4.5350

Table S2b. Molecular volume, molecular size and dipole moment of isolated nCT and isolated analytes.

	Volume (cm³ mol⁻¹)	Sizes (Å)	Dipole moment (Debye)
5CT	272.5	7.94	5.74
6CT	308.35	9.09	6.56
7CT	352.84	11.63	7.02
NH₃	23.65	1.64	1.76
N₂H₄	29.93	2.38	0.0002
HCN	30.45	2.23	3.07
H₂S	27.61	1.95	1.41
SO₂	34.18	2.52	1.99
SO₃	36.81	2.52	0.0002
CO₂	32.33	2.34	0.00
CO	33.62	1.14	0.03
H₂O₂	24.51	1.99	3.46
H₂O	12.40	1.54	2.19
CH₃OH	32.94	2.37	1.90
CH₄	23.51	1.785	0.00002