Supplementary Information

Capture and Complexation of Carbon Monoxide Using NHC and Its Boron Analogs: A Computational Study

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All possible conformers arising from different orientations of substituents such as NH_2(inward or outward due to pyramidal geometry), CHO, and COOH were fully optimized. The electronic energies in a.u of these conformers for **1**X complexes are listed below to confirm the identification of the global minimum structures discussed in the main text. The conformer selected for further analysis(global minimum) is highlighted in bold.

$1NH_2$ – CO – $1NH_2$

-786.78839789, -786.79830606, -786.80897676, -786.81315588, -786.81373867, -786.80093121, -786.79810997, -786.79035764, -786.80207426, **-786.81437558,** -786.80260335, -786.80874886

1COOH – CO – 1COOH

-1319.82662474, -1319.82509029… In all other configurations, the COOH group from the NHC ring connected to O atom is dislocated.

1CHO – CO – 1CHO

-1018.82360597, -1018.83528748, -1018.85168740, -1018.85510927, -1018.82946501, -1018.85939630, -1018.79167999, -1018.85759350, -1018.83946542, -1018.81651044, -1018.85642412, **-1018.86291643**, -1018.81983973, -1018.83714702, -1018.80960120, -1018.80995211

$1NO_2$ – CO – $1NH_2$

-1085.12836168, -1085.12098714, -1085.12497587, **-1085.13100452**, -1085.06737775, -1085.07836049, -1085.07836049, -1085.06737769

1CHO – CO – $1CH_3$

-870.82617780, -870.81864161, -870.81915297, **-870.82743115**

1CHO – CO – $1NH_2$

-902.82323127, -902.80166536, -902.80271120, -902.82320036, -902.81481644, -902.82325089, -902.79995166, -902.79301671, -902.77809114, -902.80188051, -902.81044001, -902.78844062, -902.81105140, -902.81219885, -902.85662677, -902.86074652, -902.85422618, -902.85189484, -902.84661124, -902.85212853, -902.85180907, -902.85518484,

-902.84554352, -902.85212859, -902.83598047, **-902.86250369**, -902.85518454, -902.85189485, -902.85662683

1COOH – CO – 1CH_3

-1021.30853768, -1021.30458571, -1021.30459438, **-1021.30903568**

1COOH – CO – 1NH_2

-1053.34369103, -1053.33498174, -1053.33449641, -1053.32695892, -1053.32712296, -1053.33493648, -1053.33646216, -1053.33068131, -1053.33068131, -1053.33806127, -1053.33776148, -1053.34302302, **-1053.34470905**, -1053.33634983

Table S1: Calculated bond distance, NBO partial charges and Wiberg bond indices (WBI) for free CO and all its complexes with 1X and 2X, along with stabilization energies. Atom numbering corresponds to that shown in Scheme 1.

SYSTEM	Stabilization Energy (kcal/mol)	Bond distance (Å) C2-O3	WBI C2-O3	WBI C1-C2/ B1-C2	WBI O3-C4/ O3-B4	q(C1)/ q(B1) (e)	q(C2) (e)	q(O3) (e)	q(C4)/ q(B4) (e)
CO	-	1.12	2.27	-	-	-	0.49	-0.49	-
1H-CO-1H	21.54	1.55	0.67	1.77	1.25	0.23	-0.36	-0.55	0.82
1CH_3 – CO – 1CH_3	32.39	1.54	0.68	1.78	1.24	0.23	-0.34	-0.56	0.86
1NH_2 – CO – 1NH_2	22.89	1.52	0.71	1.83	1.18	0.22	-0.28	-0.56	0.88
1COOH – CO – 1COOH	15.00	1.49	0.73	1.85	1.27	0.19	-0.10	-0.49	0.91
1CHO – CO – 1CHO	11.13	1.46	0.77	1.80	1.26	0.24	-0.22	-0.48	0.88
1NO_2 – CO – 1NO_2	28.32	1.51	0.70	1.80	1.32	0.14	-0.04	-0.46	0.87
1NO_2 – CO – 1CH_3	0.42	1.48	0.75	1.80	1.17	0.09	-0.01	-0.55	0.85
1NO_2 – CO – 1NH_2	0.40	1.49	0.74	1.81	1.17	0.09	-0.03	-0.56	0.83
1CHO – CO – 1CH_3	4.64	1.48	0.74	1.84	1.19	0.18	-0.14	-0.54	0.87
1CHO – CO – 1NH_2	1.52	1.48	0.77	1.84	1.16	0.21	-0.19	-0.54	0.81

1COOH – CO – 1CH_3	**8.44**	**1.50**	**0.72**	**1.84**	**1.19**	**0.17**	**-0.11**	**-0.55**	**0.86**
1COOH – CO – 1NH_2	**5.01**	**1.48**	**0.76**	**1.84**	**1.17**	**0.21**	**-0.16**	**-0.54**	**0.82**
2H – CO – 2H	**0.58**	**1.32**	**1.21**	**1.03**	**0.77**	**0.57**	**-0.02**	**-0.71**	**0.99**
2CH_3 – CO – 2CH_3	**3.92**	**1.40**	**0.99**	**1.17**	**0.85**	**0.64**	**-0.26**	**-0.77**	**1.11**
2NH_2 – CO – 2NH_2	**8.91**	**1.50**	**0.78**	**1.56**	**0.98**	**0.52**	**-0.68**	**-0.83**	**1.06**
2CHO – CO – 2CHO	**-4.24**	**1.53**	**0.74**	**1.80**	**1.13**	**0.54**	**-0.74**	**-0.78**	**1.16**
2NO_2 – CO – 2NO_2	**2.65**	**1.41**	**0.84**	**1.76**	**1.16**	**0.40**	**-0.37**	**-0.66**	**1.08**
2NO_2 – CO – 2CH_3	**-11.39**	**1.45**	**0.85**	**1.67**	**0.98**	**0.39**	**-0.47**	**-0.79**	**1.12**
2NO_2 – CO – 2NH_2	**-14.34**	**1.46**	**0.84**	**1.66**	**0.96**	**0.42**	**-0.49**	**-0.79**	**1.07**
2CHO – CO – 2CH_3	**-0.88**	**1.49**	**0.78**	**1.82**	**1.00**	**0.47**	**-0.69**	**-0.82**	**1.13**
2CHO – CO – 2NH_2	**-5.19**	**1.52**	**0.78**	**1.78**	**1.02**	**0.50**	**-0.66**	**-0.80**	**1.03**
2COOH – CO – 2CH_3	**3.97**	**1.48**	**0.80**	**1.85**	**1.01**	**0.44**	**-0.61**	**-0.80**	**1.12**
2COOH – CO – 2NH_2	**-0.97**	**1.54**	**0.73**	**1.81**	**0.96**	**0.48**	**-0.62**	**-0.81**	**1.07**
1H – CO – 2H	**-58.67**	**1.47**	**0.81**	**1.86**	**0.95**	**0.15**	**-0.28**	**-0.80**	**1.09**
1CH_3 – CO – 2CH_3	**-53.06**	**1.45**	**0.83**	**1.85**	**0.94**	**0.17**	**-0.26**	**-0.80**	**1.13**
1NH_2 – CO – 2NH_2	**-62.08**	**1.45**	**0.84**	**1.84**	**0.91**	**0.14**	**-0.26**	**-0.80**	**1.07**
1COOH – CO – 2COOH	**-53.90**	**1.46**	**0.81**	**1.81**	**1.02**	**0.15**	**-0.09**	**-0.77**	**1.23**
1CHO – CO – 2CHO	**-77.74**	**1.42**	**0.87**	**1.81**	**0.98**	**0.16**	**-0.14**	**-0.75**	**1.19**
1NO_2 – CO – 2NO_2	**-72.29**	**1.42**	**0.83**	**1.75**	**1.07**	**0.06**	**0.07**	**-0.73**	**1.17**
1NO_2 – CO – 2CH_3	**-99.85**	**1.40**	**0.94**	**1.69**	**0.87**	**0.05**	**-0.00**	**-0.76**	**1.12**
1NO_2 – CO – 2NH_2	**-97.19**	**1.40**	**0.94**	**1.70**	**0.87**	**0.06**	**-0.02**	**-0.76**	**1.06**
1CHO – CO – 2CH_3	**-91.00**	**1.42**	**0.88**	**1.82**	**0.89**	**0.16**	**-0.16**	**-0.79**	**1.12**
1CHO – CO – 2NH_2	**-88.28**	**1.43**	**0.88**	**1.81**	**0.89**	**0.17**	**-0.18**	**-0.78**	**1.06**
1COOH – CO – 2CH_3	**-82.62**	**1.41**	**0.90**	**1.79**	**0.90**	**0.12**	**-0.08**	**-0.77**	**1.12**
1COOH – CO – 2NH_2	**-81.69**	**1.42**	**0.90**	**1.79**	**0.89**	**0.13**	**-0.10**	**-0.77**	**1.06**

Table S2: Electron Localization Function values at the bond critical points of CO, C-C/B-C, and O-C/O-B bonds for free CO and its most stable complexes with 1X and 2X.

SYSTEM	Electron Localization Function (ELF)		
	C2-O3	C1-C2/B1-C2	O3-C4/O3-B4
CO	0.39	-	-
$1NO_2$ – CO – $1CH_3$	0.41	0.92	0.54
$1NO_2$ – CO – $1NH_2$	0.42	0.92	0.54
2H – CO – 2H	0.38	0.62	0.21
2CHO – CO – 2CHO	0.41	0.50	0.22
$2NO_2$ – CO – $2CH_3$	0.39	0.51	0.22
$2NO_2$ – CO – $2NH_2$	0.41	0.50	0.26
2CHO – CO – $2CH_3$	0.41	0.49	0.22
2CHO – CO – $2NH_2$	0.44	0.49	0.22
2COOH – CO – $2NH_2$	0.46	0.49	0.22
1H – CO – 2H	0.43	0.90	0.22
$1CH_3$ – CO – $2CH_3$	0.44	0.91	0.19
$1NH_2$ – CO – $2NH_2$	0.47	0.92	0.19
1COOH – CO – 2COOH	0.42	0.92	0.20
1CHO – CO – 2CHO	0.41	0.91	0.19
$1NO_2$ – CO – $2NO_2$	0.36	0.92	0.18
$1NO_2$ – CO – $2CH_3$	0.42	0.93	0.19
$1NO_2$ – CO – $2NH_2$	0.48	0.93	0.23
1CHO – CO – $2CH_3$	0.43	0.91	0.19
1CHO – CO – $2NH_2$	0.44	0.91	0.19
1COOH – CO – $2CH_3$	0.43	0.92	0.19
1COOH – CO – $2NH_2$	0.45	0.92	0.19

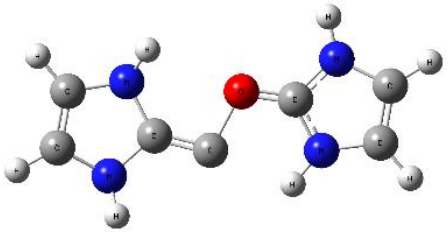
Table S3: Electron density ρ(r) and energy density H(r) values for C-O, C-C/B-C, and O-C/O-B bonds for free CO and its most stable complexes with 1X and 2X.

SYSTEM	$\rho(r_{C-O})$	$H(r_{C-O})$	ρ $(r_{c-c}/_{B-C})$	H $(r_{c-c}/_{B-C})$	ρ $(r_{O-c}/_{O-B})$	H $(r_{O-c}/_{O-B})$
CO	**0.487**	**-0.852**	**-**	**-**	**-**	**-**
$1NO_2$ – CO – $1CH_3$	**0.194**	**-0.234**	**0.341**	**-0.398**	**0.347**	**-0.542**
$1NO_2$ – CO – $1NH_2$	**0.192**	**-0.230**	**0.341**	**-0.399**	**0.348**	**-0.544**
2H – CO – 2H	**0.287**	**-0.407**	**0.188**	**-0.196**	**0.182**	**-0.138**
2CHO – CO – 2CHO	**0.167**	**-0.179**	**0.219**	**-0.242**	**0.243**	**-0.218**
$2NO_2$ – CO – $2CH_3$	**0.211**	**-0.265**	**0.216**	**-0.238**	**0.222**	**-0.191**
$2NO_2$ – CO – $2NH_2$	**0.207**	**-0.256**	**0.217**	**-0.239**	**0.220**	**-0.188**
2CHO – CO – $2CH_3$	**0.182**	**-0.208**	**0.219**	**-0.241**	**0.226**	**-0.196**
2CHO – CO – $2NH_2$	**0.179**	**-0.200**	**0.219**	**-0.241**	**0.225**	**-0.195**
2COOH – CO – $2NH_2$	**0.170**	**-0.180**	**0.217**	**-0.237**	**0.219**	**-0.186**
1H – CO – 2H	**0.205**	**-0.254**	**0.336**	**-0.403**	**0.216**	**-0.182**
$1CH_3$ – CO – $2CH_3$	**0.212**	**-0.273**	**0.324**	**-0.344**	**0.208**	**-0.128**
$1NH_2$ – CO – $2NH_2$	**0.212**	**-0.271**	**0.326**	**-0.343**	**0.205**	**-0.126**
1COOH – CO – 2COOH	**0.205**	**-0.259**	**0.329**	**-0.348**	**0.228**	**-0.146**
1CHO – CO – 2CHO	**0.225**	**-0.307**	**0.329**	**-0.353**	**0.219**	**-0.137**
$1NO_2$ – CO – $2NO_2$	**0.217**	**-0.293**	**0.330**	**-0.345**	**0.227**	**-0.138**
$1NO_2$ – CO – $2CH_3$	**0.245**	**-0.352**	**0.326**	**-0.338**	**0.198**	**-0.119**
$1NO_2$ – CO – $2NH_2$	**0.249**	**-0.334**	**0.332**	**-0.373**	**0.203**	**-0.168**
1CHO – CO – $2CH_3$	**0.227**	**-0.310**	**0.327**	**-0.355**	**0.200**	**-0.121**
1CHO – CO – $2NH_2$	**0.226**	**-0.306**	**0.328**	**-0.355**	**0.201**	**-0.122**
1COOH – CO – $2CH_3$	**0.234**	**-0.325**	**0.328**	**-0.347**	**0.203**	**-0.124**
1COOH – CO – $2NH_2$	**0.235**	**-0.326**	**0.328**	**-0.350**	**0.202**	**-0.123**

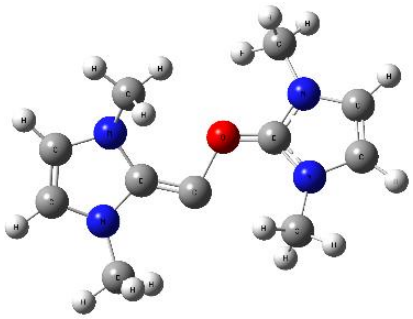
Table S4: Stabilization energies (kcal/mol) for complexes of CO with 1X and 2X ligands in the presence of different protic, aprotic, and non-polar solvents, including water.

Complex	Stabilization Energy in different solvents (kcal/mol)			
	Methanol	THF	Toluene	Water
2H – CO – 2H	-40.79	-31.73	-10.02	-42.45
2CHO – CO – 2CHO	-58.86	-53.37	-38.87	-59.67
$2NO_2$ – CO – $2CH_3$	-69.56	-63.79	-49.03	-70.66
$2NO_2$ – CO – $2NH_2$	-70.28	-65.03	-51.07	-71.21
2CHO – CO – $2NH_2$	-59.96	-54.58	-40.36	-60.92
2COOH – CO – $2NH_2$	-60.88	-56.23	-34.72	-62.36
1H – CO – 2H	-52.34	-53.98	-58.36	-52.07
$1CH_3$ – CO – $2CH_3$	-47.21	-47.56	-53.33	46.96
$1NH_2$ – CO – $2NH_2$	-54.13	-56.31	-61.88	-53.76
1COOH – CO – 2COOH	-57.75	-57.92	-59.36	-57.75
1CHO – CO – 2CHO	-71.27	-73.19	-77.96	-70.93
$1NO_2$ – CO – $2NO_2$	-71.45	-72.86	-76.31	-71.20
$1NO_2$ – CO – $2CH_3$	-89.55	-92.36	-99.90	-88.99
$1NO_2$ – CO – $2NH_2$	-86.84	-89.80	-96.74	-86.30
1CHO – CO – $2CH_3$	-78.98	-82.37	-89.90	-78.40
1CHO – CO – $2NH_2$	-76.92	-79.86	-86.74	-76.38
1COOH – CO – $2CH_3$	-72.54	-75.18	-81.83	-72.10
1COOH – CO – $2NH_2$	-71.62	-73.99	-80.19	-71.23

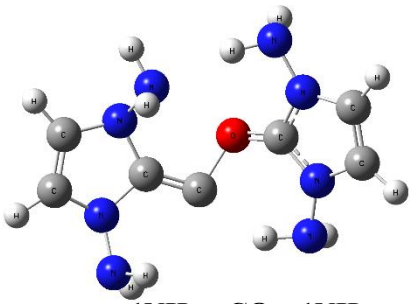
Figure S1: Computed structures of CO complexes with 1X and 2X ligands.



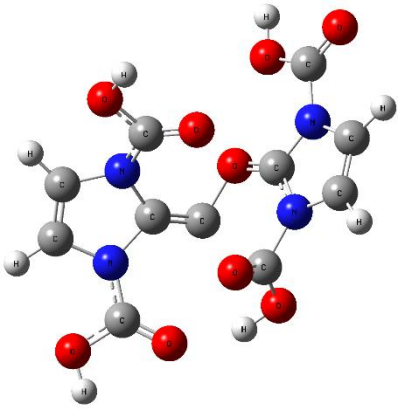
1H – CO – 1H



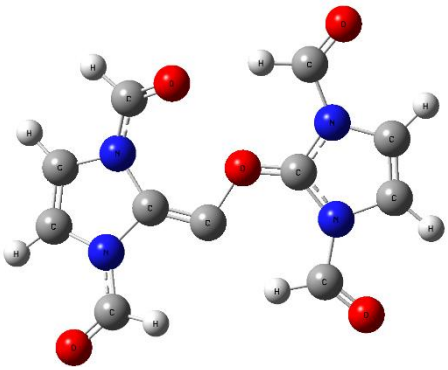
$1CH_3$ – CO – $1CH_3$



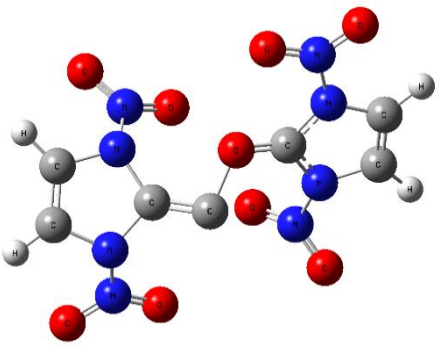
$1NH_2$ – CO – $1NH_2$



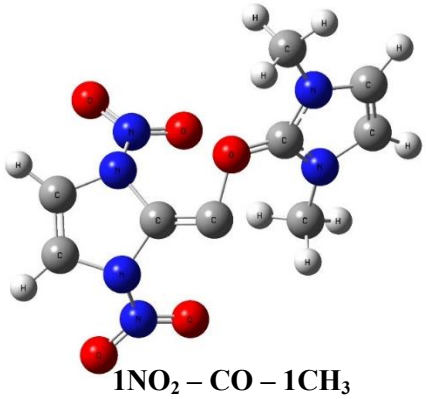
1COOH – CO – 1COOH



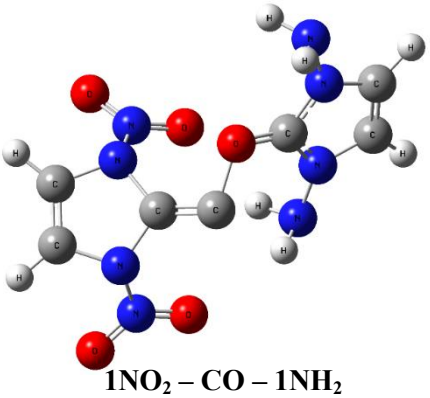
1CHO – CO – 1CHO



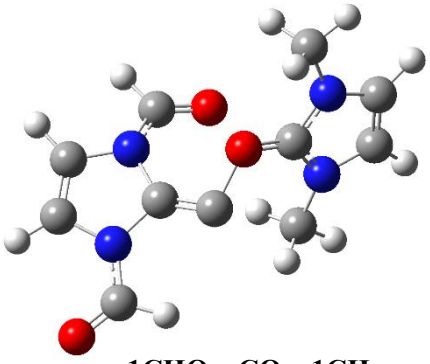
$1NO_2$ – CO – $1NO_2$



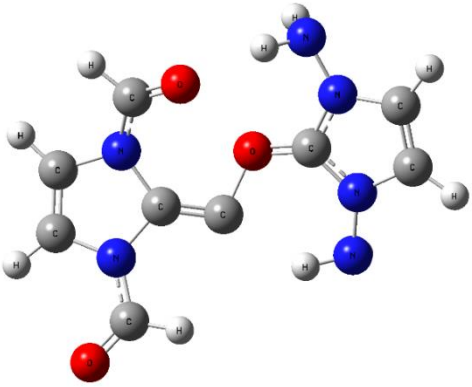
$1NO_2$ – CO – $1CH_3$



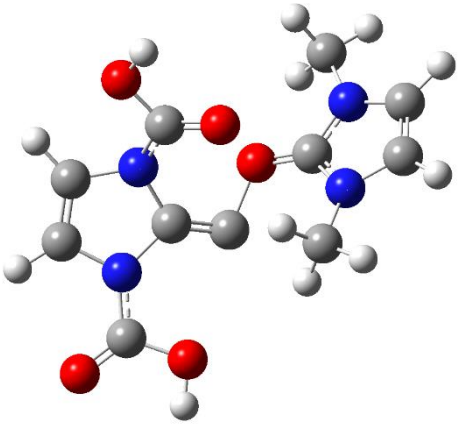
$1NO_2$ – CO – $1NH_2$



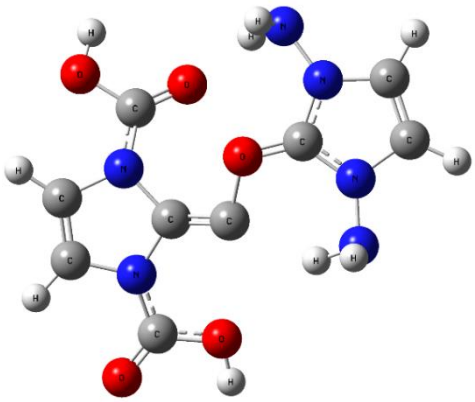
1CHO – CO – $1CH_3$



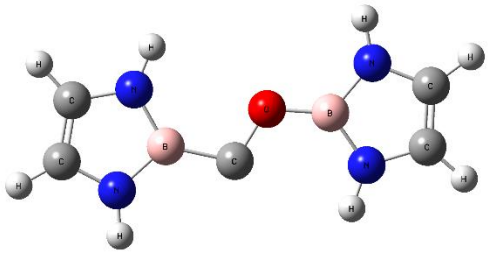
1CHO – CO – $1NH_2$



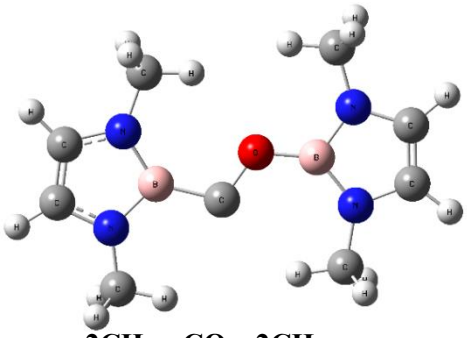
1COOH – CO – $1CH_3$



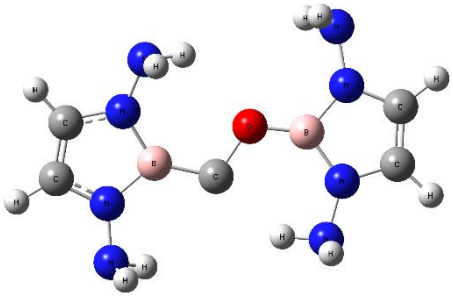
1COOH – CO – $1NH_2$



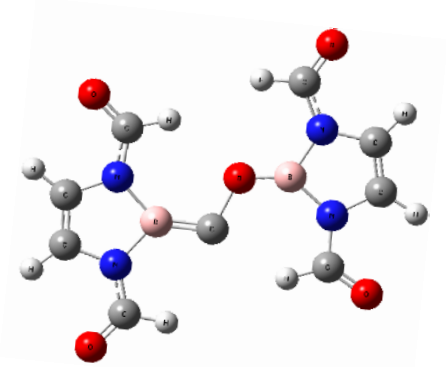
2H – CO – 2H



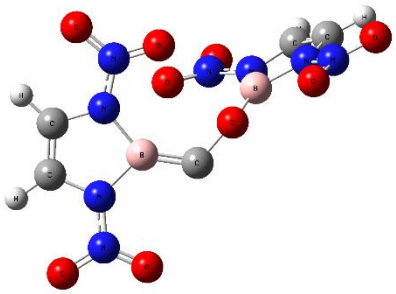
$2CH_3$ – CO – $2CH_3$



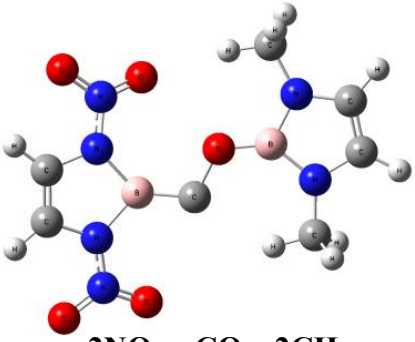
$2NH_2$ – CO – $2NH_2$



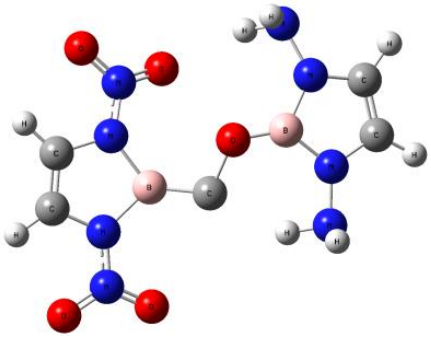
2CHO – CO – 2CHO



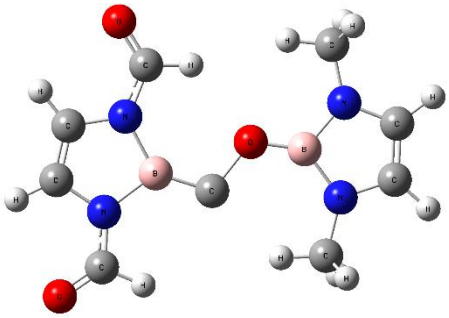
$2NO_2$ – CO – $2NO_2$



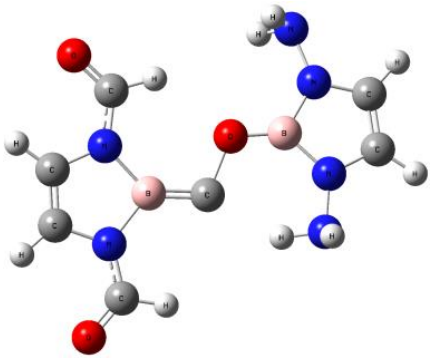
$2NO_2$ – CO – $2CH_3$



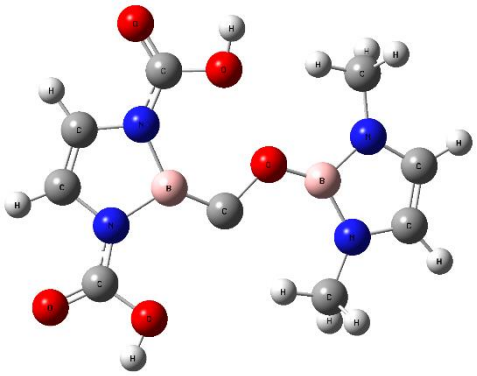
$2NO_2$ – CO – $2NH_2$



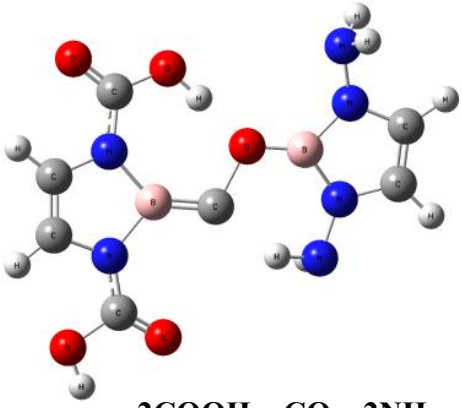
2CHO – CO – $2CH_3$



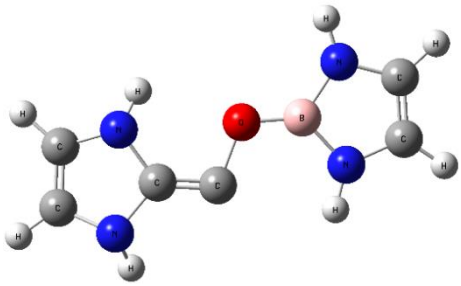
2CHO – CO – $2NH_2$



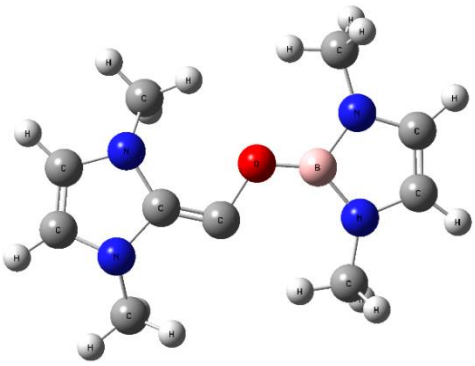
2COOH – CO – $2CH_3$



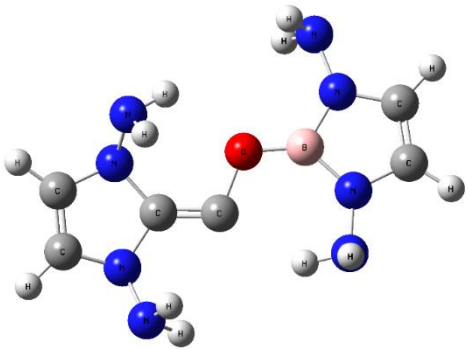
2COOH – CO – $2NH_2$



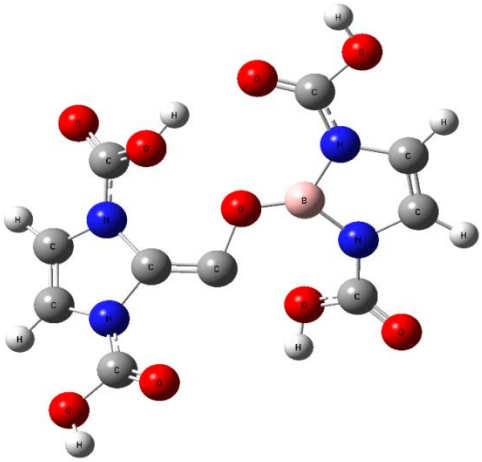
1H – CO – 2H



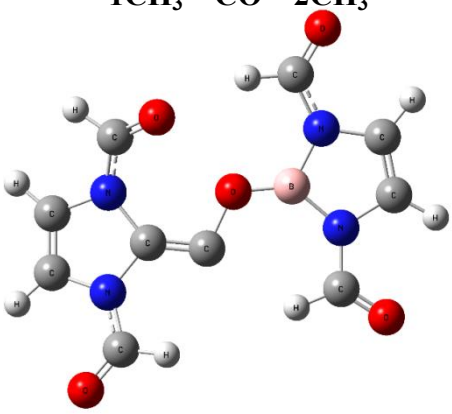
1CH_3 – CO – 2CH_3



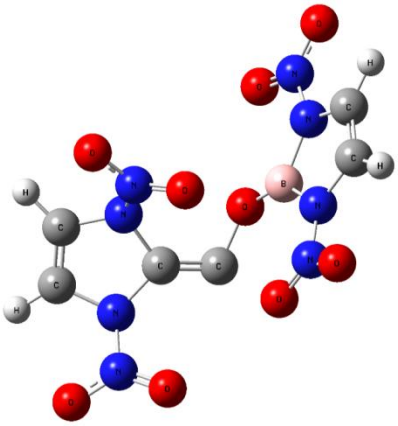
1NH_2 – CO – 2NH_2



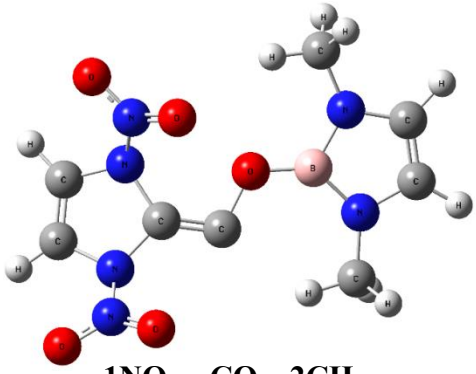
1COOH – CO – 2COOH



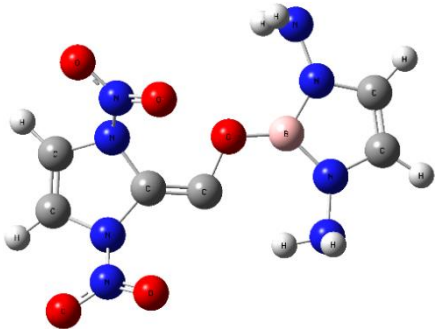
1CHO – CO – 2CHO



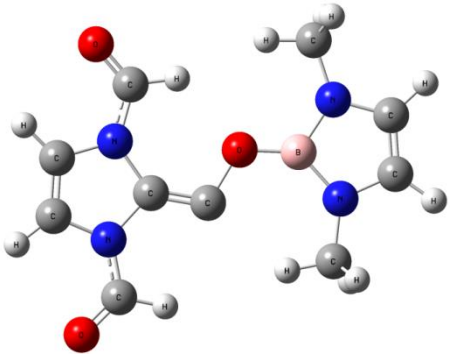
1NO_2 – CO – 2NO_2



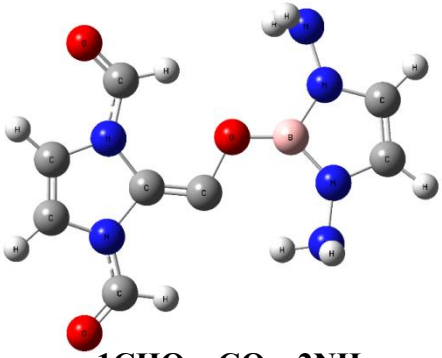
1NO_2 – CO – 2CH_3



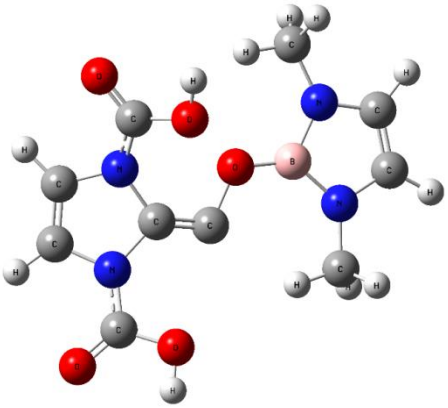
1NO_2 – CO – 2NH_2



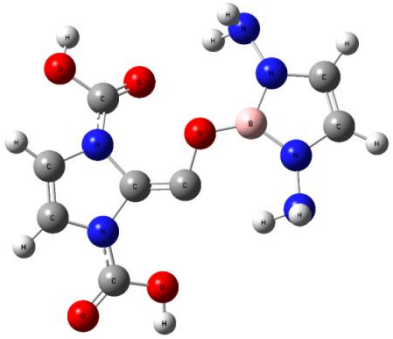
1CHO – CO – 2CH_3



1CHO – CO – 2NH_2



1COOH – CO – 2CH_3



1COOH – CO – 2NH_2

Figure S2: Electron Localization Function (ELF) plots of the CO unit in the complex $1NO_2$ – CO – $1CH_3$. The C-C-O and C-O-C bonding regions are shown separately because they lie in different molecular planes.

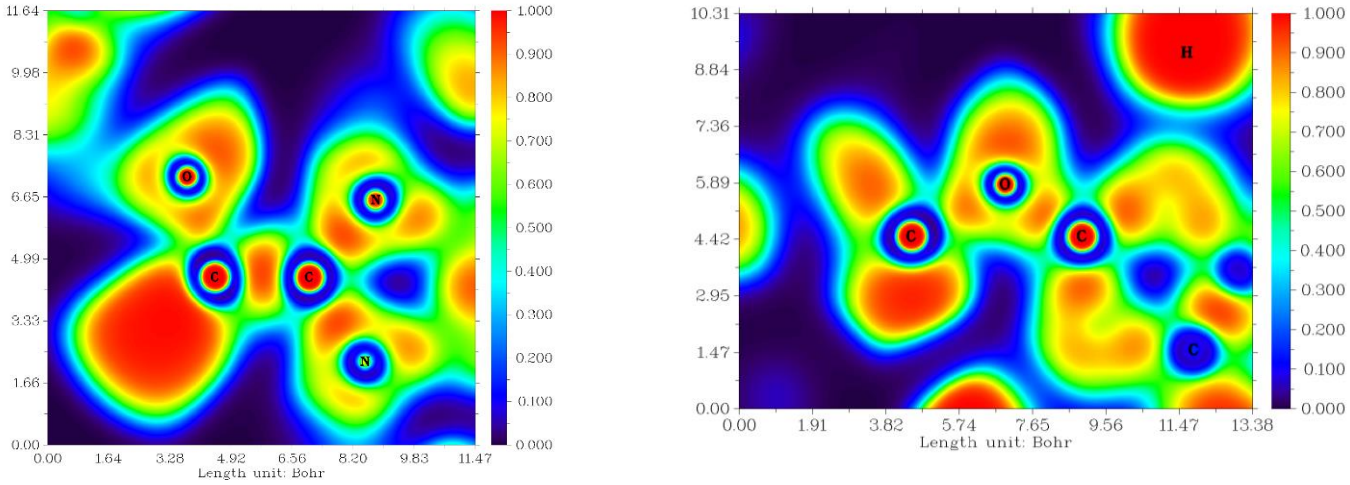
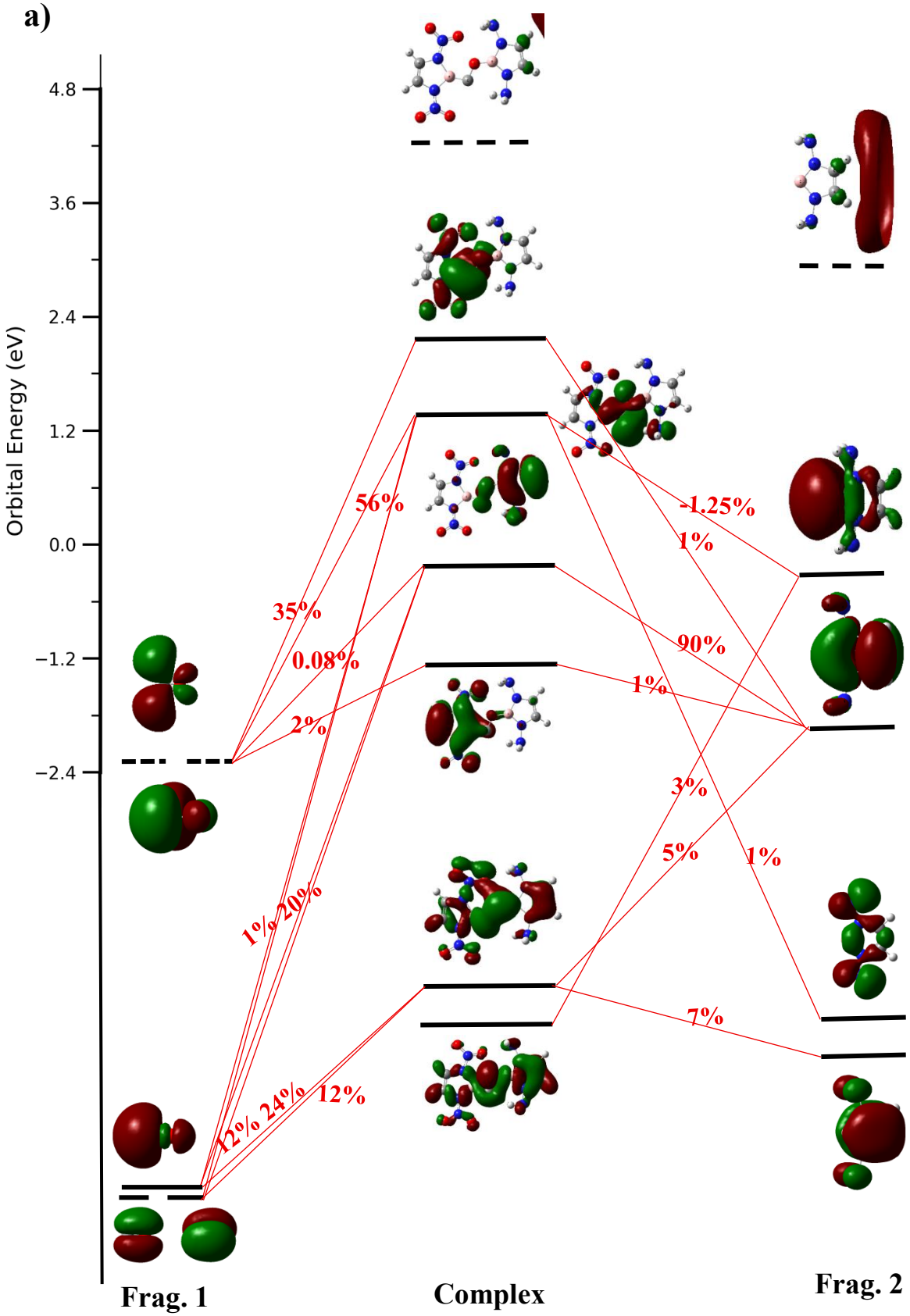


Figure S3: CDA orbital interaction diagrams for the complex $2NO_2$ - CO - $2NH_2$. The diagrams represent pairwise fragment interactions: (a) CO (Frag. 1) with $2NH_2$ (Frag. 2), and (b) $2NO_2$ (Frag. 3) with CO (Frag. 1). Red lines indicate orbital mixing between fragments, and the percentage values represent the contribution of each fragment orbital to the corresponding molecular orbitals of the complex.


a)
Orbital Energy (eV)
4.8
3.6
2.4
1.2
0.0
−1.2
−2.4
56%
35%
0.08%
2%
1%
20%
12%
24%
12%
-1.25%
1%
90%
1%
3%
5%
1%
7%
Frag. 1
Complex
Frag. 2

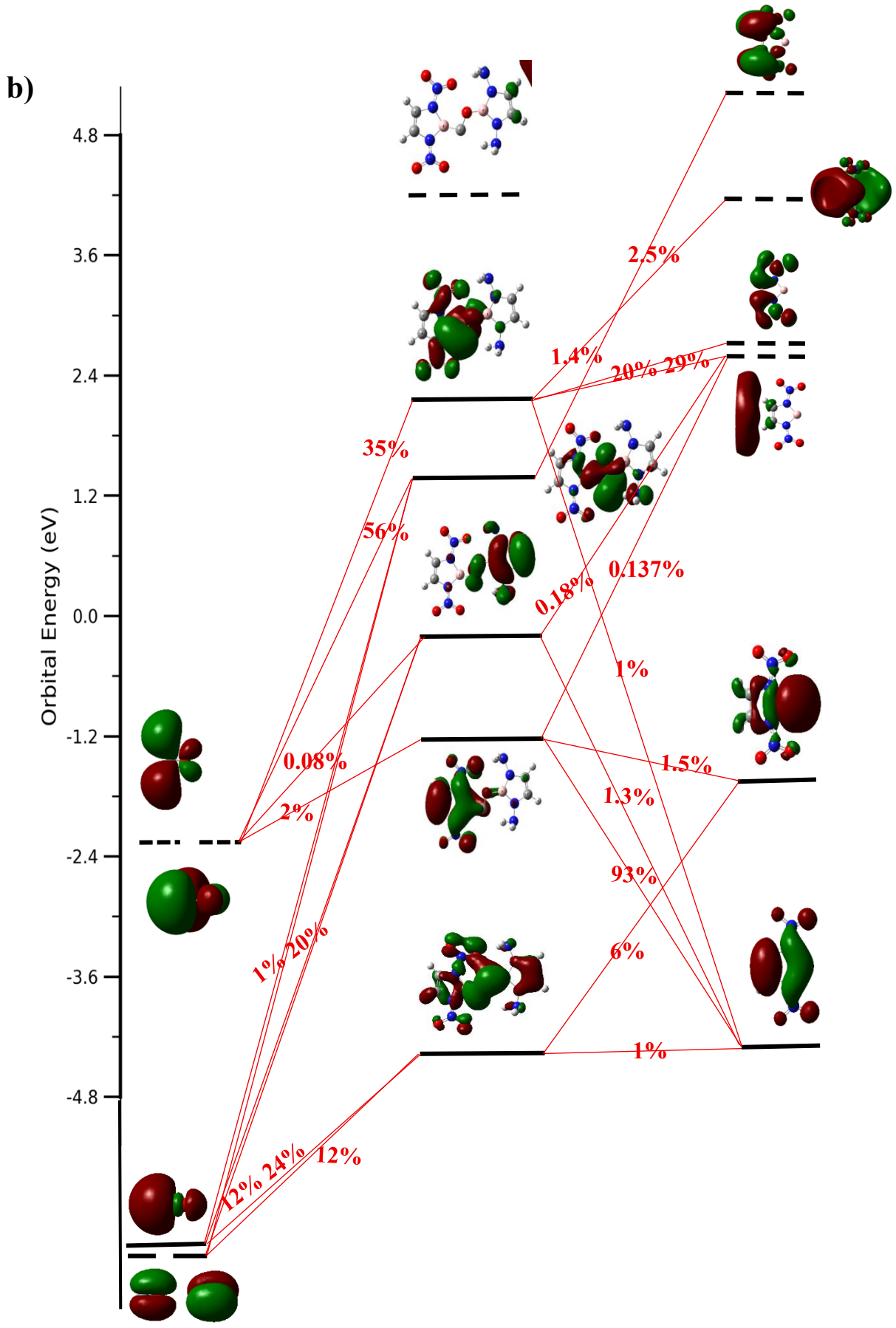
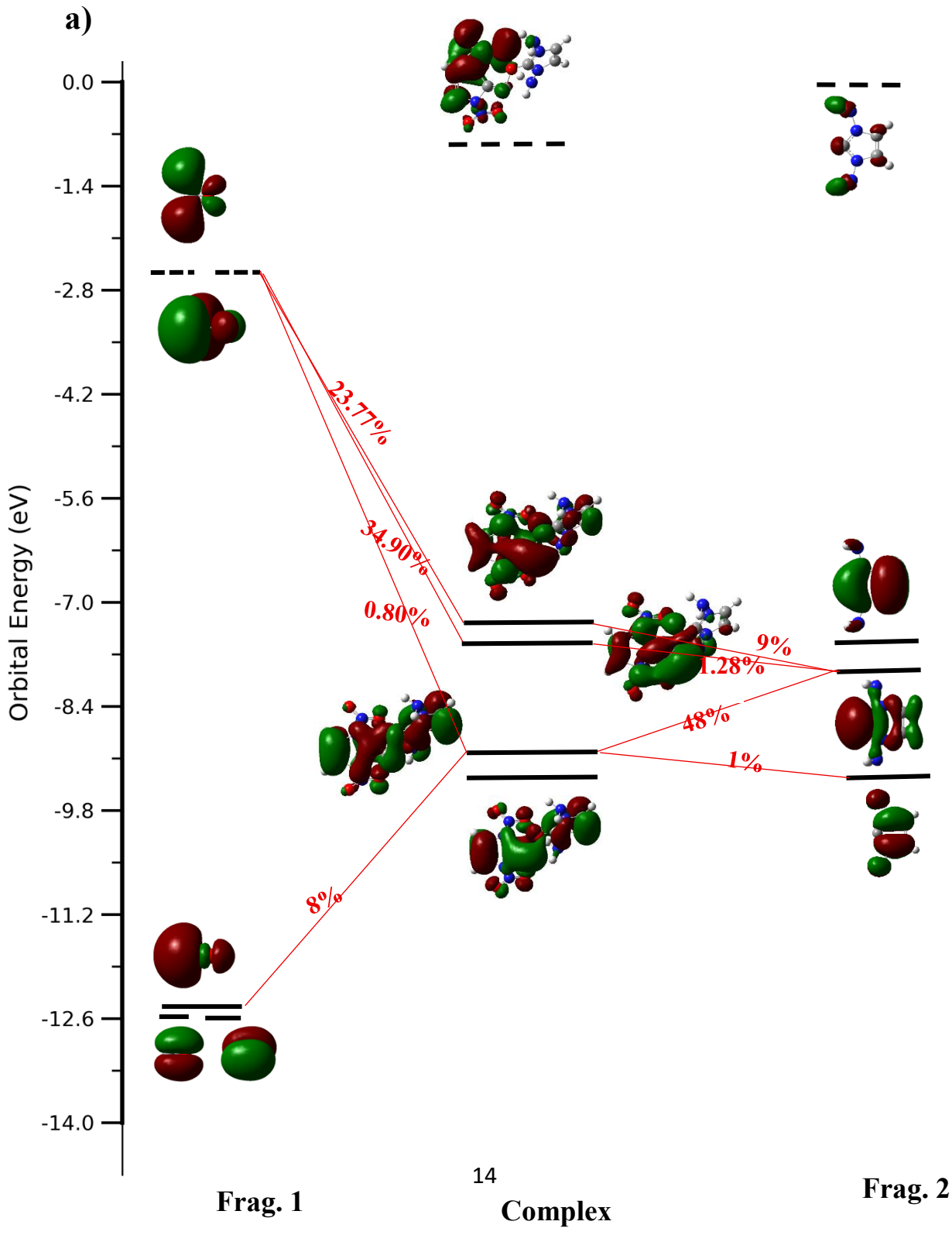

b)
Orbital Energy (eV)
4.8
3.6
2.4
1.2
0.0
-1.2
-2.4
-3.6
-4.8
2.5%
1.4%
20% 29%
35%
56%
0.18%
0.137%
1%
0.08%
2%
1.5%
1.3%
93%
1% 20%
6%
1%
12% 24% 12%
Frag. 1
Complex
Frag. 3

Figure S4: CDA orbital interaction diagrams for the complex $1NO_2$ - CO - $1NH_2$. The diagrams represent pairwise fragment interactions: (a) CO (Frag. 1) with $1NH_2$ (Frag. 2), and (b) $1NO_2$ (Frag. 3) with CO (Frag. 1). Red lines indicate orbital mixing between fragments, and the percentage values represent the contribution of each fragment orbital to the corresponding molecular orbitals of the complex.



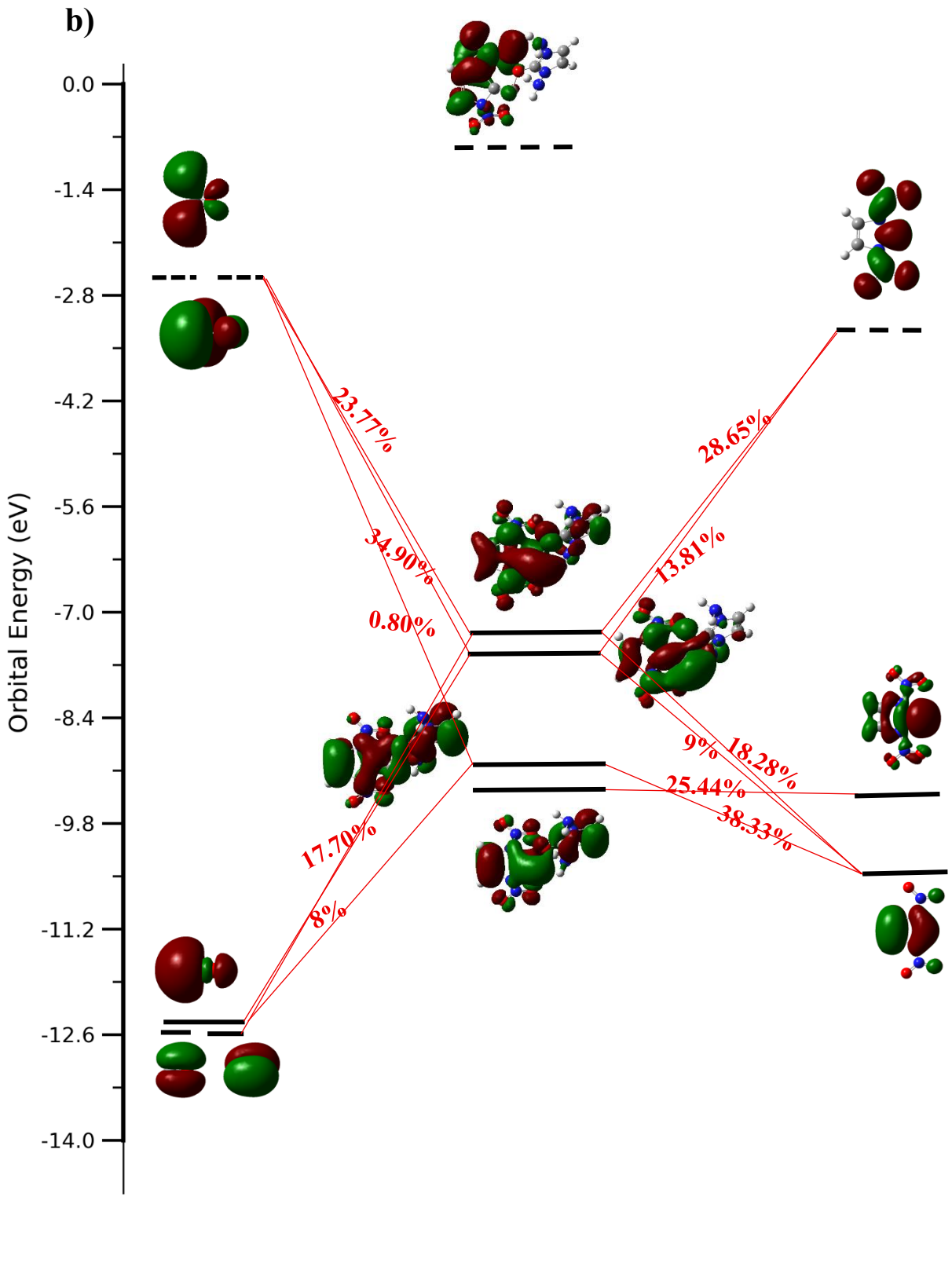
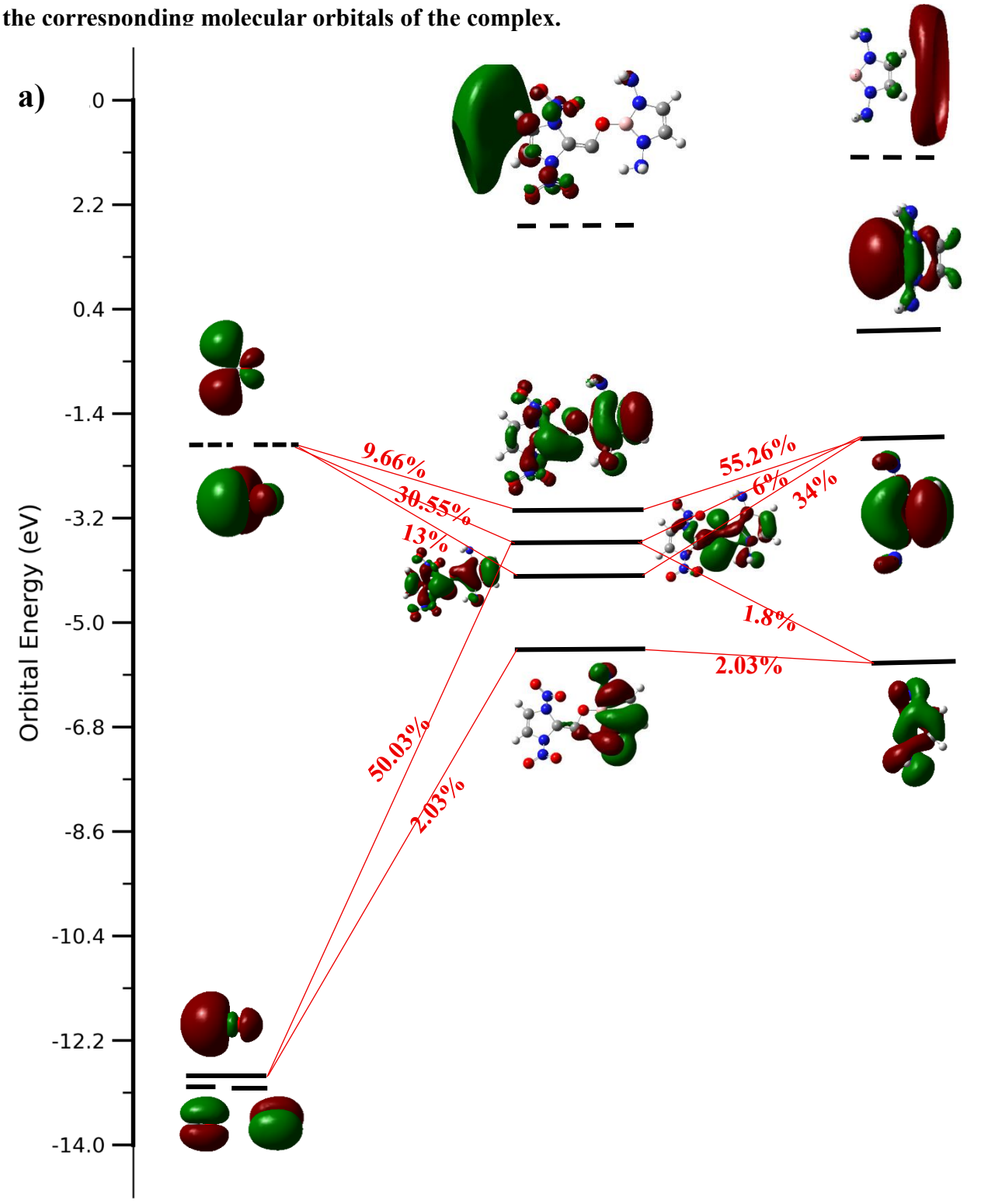

b)
0.0
-1.4
-2.8
-4.2
-5.6
-7.0
-8.4
-9.8
-11.2
-12.6
-14.0
Orbital Energy (eV)
23.77%
34.90%
0.80%
17.70%
8%
28.65%
13.81%
9%
18.28%
25.44%
38.33%
Frag. 1
Complex
Frag. 2

Figure S5: CDA orbital interaction diagrams for the complex $1NO_2$ - CO - $2NH_2$. The diagrams represent pairwise fragment interactions: (a) CO (Frag. 1) with $2NH_2$ (Frag. 2), and (b) $1NO_2$ (Frag. 3) with CO (Frag. 1). Red lines indicate orbital mixing between fragments, and the percentage values represent the contribution of each fragment orbital to the corresponding molecular orbitals of the complex.



b)

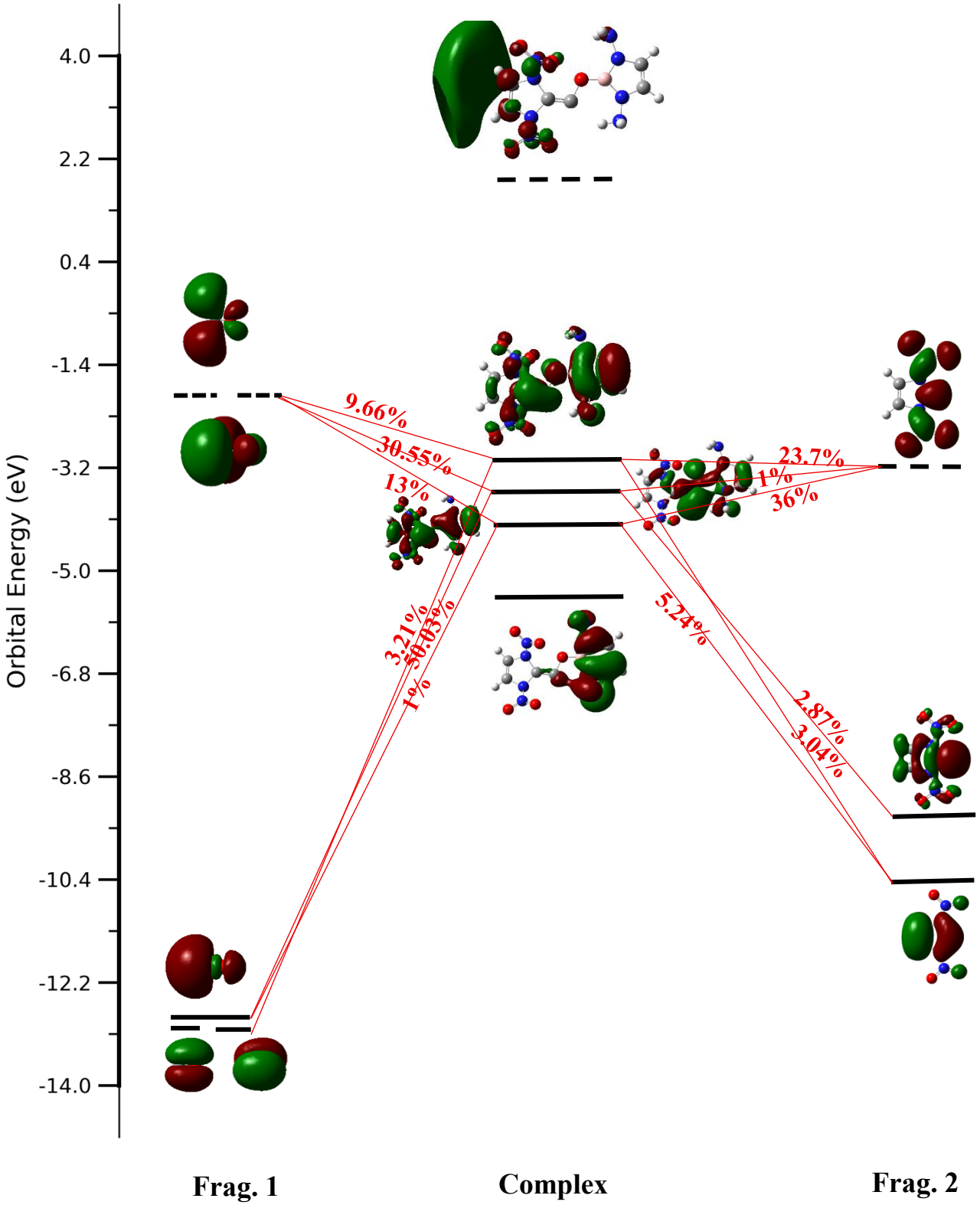
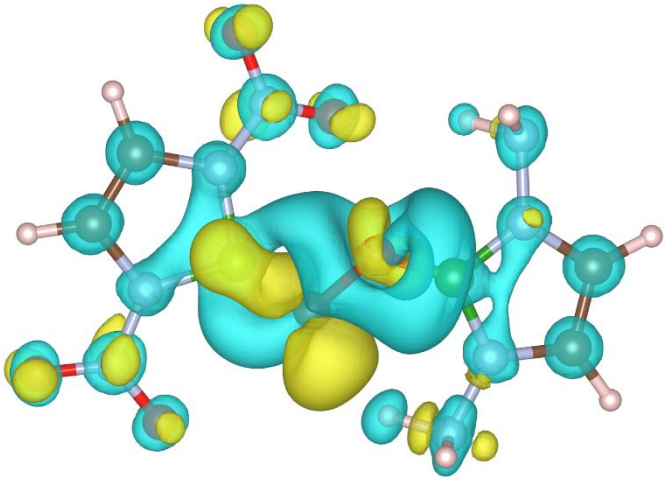
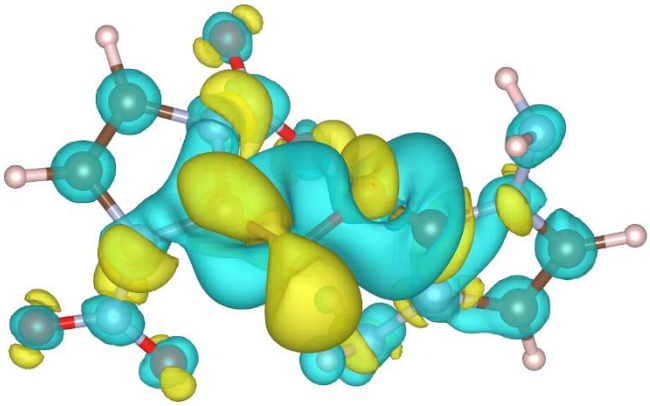

4.0
2.2
0.4
-1.4
-3.2
-5.0
-6.8
-8.6
-10.4
-12.2
-14.0
Orbital Energy (eV)
9.66%
30.55%
13%
3.21%
50.03%
1%
23.7%
1%
36%
5.24%
2.87%
3.04%
Frag. 1
Complex
Frag. 2

Figure S6: Charge density difference (CDD) plot of the complex $2NO_2 – CO – 2NH_2$. Yellow regions indicate electron accumulation, while blue regions represent electron depletion upon complex formation.

a)



b)



c)

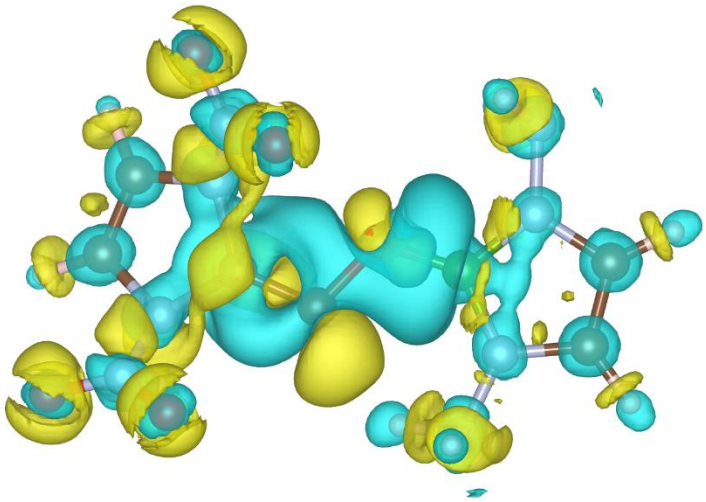
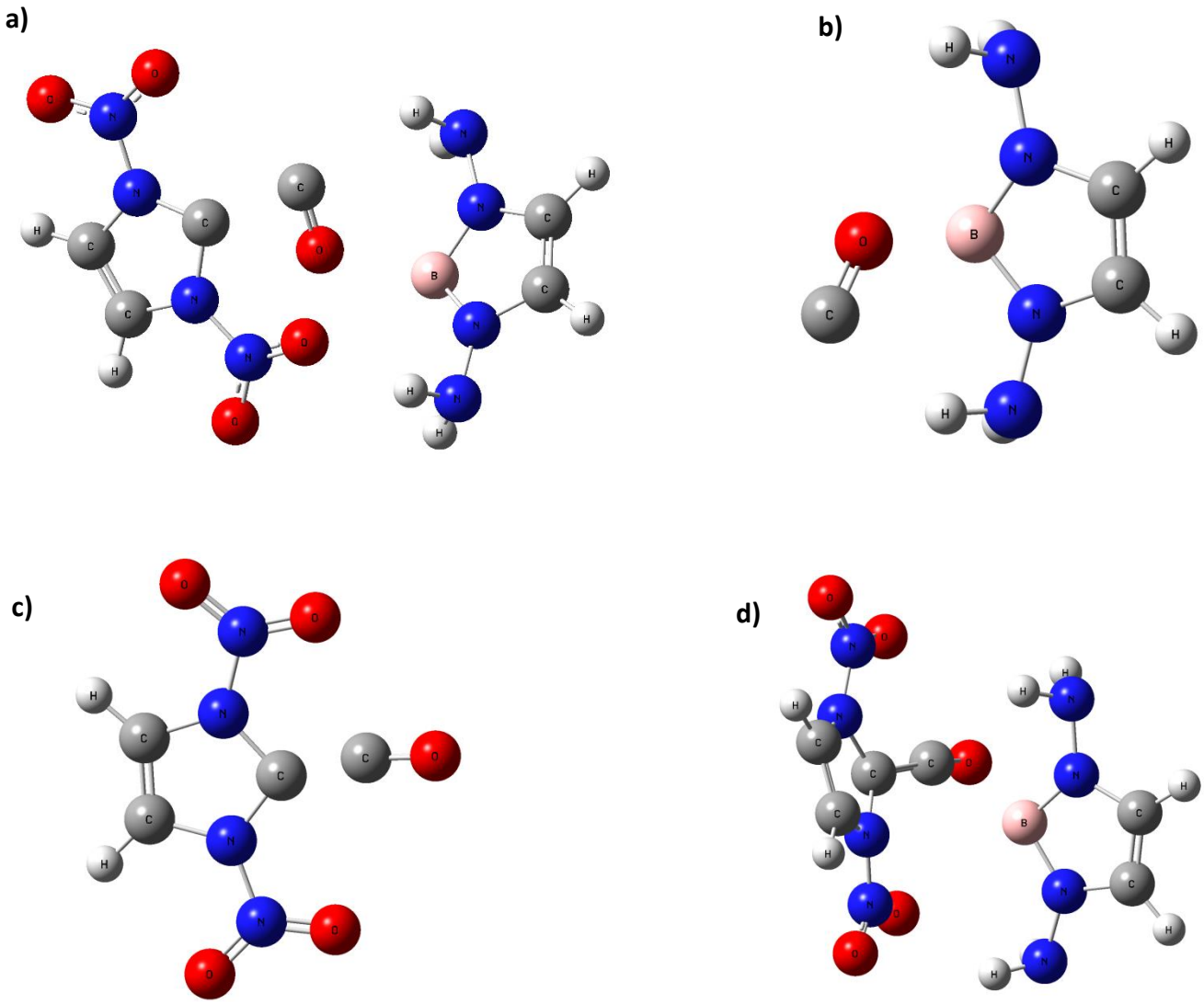


Figure S7: Transition state structures for the possible reaction pathways of $1NO_2$ – CO – $2NH_2$: (a) concerted mechanism, (b) first transition state corresponding to initial coordination at the oxygen end of CO with $2NH_2$, (c) first transition state corresponding to initial coordination at the carbon end of CO with $1NO_2$, and (d) second transition state involving coordination of $2NH_2$ through B-O bond formation with the intermediate.



Cartesian coordinates of computed complexes

1. 1H-CO-1H

Charge = 0 Multiplicity = 1

C	3.570199	-0.921314	0.021932
C	3.915979	0.388173	0.024640
H	4.190574	-1.805937	0.026813
H	4.885664	0.864656	0.032652
C	-1.672789	-0.306133	-0.099195
C	-3.584944	0.927716	0.101886
C	-3.940913	-0.366489	0.134885
H	-4.207374	1.812686	0.141929
H	-4.927292	-0.804738	0.220040
N	2.728240	1.122966	0.015817
H	2.629363	2.126161	0.007057
N	2.184067	-0.980228	0.009176
H	1.446040	-1.708307	0.006662
N	-2.204215	1.004277	-0.185478
H	-1.644943	1.743683	0.215250
N	-2.805974	-1.152616	-0.128661
H	-2.701894	-2.066052	0.289413
C	1.683631	0.261059	0.004758
C	-0.396200	-0.746528	0.000699
O	0.445657	0.557269	-0.006678

2. $1CH_3 – CO – 1CH_3$

Charge = 0 Multiplicity = 1

C	-3.695373	1.013953	0.155293
C	-3.955608	-0.257891	-0.225434
H	-4.363694	1.841472	0.348420
H	-4.890154	-0.761465	-0.429589
C	1.724426	0.088591	-0.192919
C	3.561602	-1.210126	0.201353
C	4.001295	0.011454	-0.149125
H	4.124358	-2.107082	0.428156
H	5.015583	0.372347	-0.270735
N	-2.732813	-0.898513	-0.342999
N	-2.318257	1.154858	0.284855
N	2.151222	-1.242134	0.099009
N	2.909706	0.796487	-0.492512
C	-1.740360	-0.031166	-0.020493
C	0.517042	0.720663	-0.213613
O	-0.522190	-0.395663	-0.031020
C	1.429561	-2.027042	1.085478
H	0.506446	-2.437529	0.667212
H	2.072029	-2.857401	1.398269
H	1.177369	-1.414904	1.967945
C	2.910185	2.233085	-0.545766
H	3.915823	2.577029	-0.811165
H	2.189675	2.565497	-1.302252
H	2.606405	2.670083	0.421096
C	-2.483808	-2.276663	-0.723857
H	-1.553180	-2.314125	-1.297215
H	-2.389311	-2.914436	0.162791

H	-3.316983	-2.622147	-1.341413
C	-1.673867	2.381699	0.764970
H	-0.926883	2.128501	1.516962
H	-1.161002	2.882063	-0.056682
H	-2.468538	3.003175	1.192564

3. $1NH_2 – CO – 1NH_2$

Charge = 0 Multiplicity = 1

C	3.448512	0.834146	-0.703749
C	3.550044	-0.519825	-0.672307
H	4.083165	1.596291	-1.133097
H	4.288654	-1.201424	-1.068976
C	-1.629309	0.205125	0.349028
C	-3.268881	-1.302137	-0.188653
C	-3.777308	-0.073165	-0.368297
H	-3.752555	-2.268610	-0.266432
H	-4.765350	0.239582	-0.684159
N	2.437447	-0.984129	0.009974
N	2.286700	1.176492	-0.030783
N	-1.939063	-1.201244	0.334729
N	-2.853710	0.867170	0.055243
C	1.668008	0.057188	0.385809
C	-0.498989	0.912847	0.571251
O	0.554707	-0.085963	1.009804
N	2.066011	-2.322336	0.164798
H	2.250040	-2.581363	1.133608
H	1.042493	-2.329939	0.040663
N	-0.980585	-2.002764	-0.373966
H	-1.248336	-2.968486	-0.188525
H	-1.130136	-1.852959	-1.378105
N	1.801116	2.482960	0.137514
H	0.759314	2.322871	0.217711
H	2.106098	2.786534	1.063479
N	-2.865802	2.163162	-0.467289
H	-2.579781	2.781168	0.290991
H	-2.108525	2.223803	-1.155621

4. 1COOH – CO – 1COOH

Charge = 0 Multiplicity = 1

C	-3.299173	1.675225	-0.210093
C	-2.301473	2.473616	0.177638
H	-4.357049	1.878636	-0.292175
H	-2.327051	3.505295	0.498274
N	-2.770012	0.399172	-0.517403
N	-1.080835	1.749644	0.135432
O	-3.072622	-1.898895	-0.506158
O	0.916965	1.290048	1.200465
C	-3.489014	-0.750282	-0.506772
C	-0.027862	2.014744	0.962252
C	3.349869	-1.306711	0.752750
C	2.288260	-2.011978	1.172246
H	4.390635	-1.307918	1.041421
H	2.197373	-2.776140	1.931579
N	2.893828	-0.445611	-0.258238
N	1.178701	-1.619429	0.415740
C	3.740226	0.520291	-0.832945

C	-0.197789	-2.038885	0.755803
C	-0.605986	-0.338412	-1.309643
O	0.824593	0.057600	-1.211224
O	-0.146161	3.249185	1.509916
H	0.627858	3.356168	2.078094
O	-4.816579	-0.492167	-0.500975
H	-5.251034	-1.355234	-0.487405
O	-0.679004	-1.655853	1.779399
O	4.897756	0.603571	-0.523954
O	3.108928	1.273666	-1.725889
H	3.761873	1.898708	-2.073704
O	-0.655461	-2.901444	-0.114921
H	-1.616052	-2.679040	-0.261662
C	1.540553	-0.628890	-0.422902
C	-1.331888	0.505850	-0.557737

5. 1CHO – CO – 1CHO

Charge = 0 Multiplicity = 1

C	4.030452	-0.425343	-0.414148
C	3.460621	-1.624178	-0.558580
H	5.051621	-0.099994	-0.561631
H	3.893784	-2.569377	-0.859083
N	3.059505	0.483155	0.020987
N	2.085910	-1.533114	-0.203241
O	4.447972	2.261387	0.292559
O	0.293565	-2.706939	0.676028
C	3.338757	1.778195	0.385322
H	2.452792	2.311329	0.764669
H	1.946506	-3.567302	-0.129029
C	1.383746	-2.654472	0.141955
C	-3.922811	0.171330	-0.069201
C	-3.527169	1.453076	-0.065765
H	-4.900829	-0.290024	-0.072374
H	-4.079284	2.382343	-0.070143
N	-2.765811	-0.618543	-0.055680
N	-2.116706	1.479097	-0.054193
O	-3.764741	-2.656784	0.005254
O	-2.031211	3.751405	-0.090345
C	-2.737814	-2.042161	0.038105
H	-1.717882	-2.445499	0.151665
H	-0.307408	2.580417	-0.054836
C	-1.395604	2.739373	-0.070067
C	0.643950	0.596949	0.058101
O	-0.501598	-0.302351	-0.076346
C	-1.668449	0.191541	-0.055568
C	1.772406	-0.142611	0.012921

6. $1NO_2 – CO – 1NO_2$

Charge = 0 Multiplicity = 1

C	-3.200726	1.899845	-0.233029
C	-3.946781	0.806431	-0.007045
H	-3.469305	2.916167	-0.488692
H	-5.013276	0.634890	-0.014781
C	1.530971	-0.310751	0.586576
C	2.968793	-2.091423	0.296949
C	3.681865	-1.096042	0.828245

H	3.245092	-3.117373	0.096680
H	4.705549	-1.086827	1.176077
N	-3.050459	-0.233140	0.281524
N	-1.858984	1.531412	-0.074490
N	1.641499	-1.636749	0.031881
N	2.867911	0.060033	0.960365
C	-1.747563	0.213674	0.244778
C	0.457692	0.405200	0.962553
O	-0.730318	-0.435799	0.575270
N	1.171581	-1.903337	-1.271486
O	1.588326	-2.922486	-1.778982
O	0.354311	-1.143683	-1.737097
N	3.433066	1.269943	0.497689
O	2.676311	2.154009	0.192475
O	4.646855	1.316380	0.523905
N	-3.469851	-1.549523	0.622618
O	-4.665066	-1.687594	0.655434
O	-2.600132	-2.343376	0.824649
N	-0.797784	2.376665	-0.644700
O	-0.893751	3.522994	-0.318627
O	-0.063090	1.825104	-1.395434

7. $1NO_2 – CO – 1CH_3$

Charge = 0 Multiplicity = 1

C	-3.653942	-1.398537	0.717881
C	-4.329169	-0.414291	0.076930
H	-4.007941	-2.206702	1.342507
H	-5.385603	-0.189712	0.031268
C	2.684035	1.761518	-0.372697
C	3.347498	0.682451	-0.795947
H	3.030418	2.775912	-0.227261
H	4.385894	0.580687	-1.081040
N	-3.387022	0.346960	-0.594607
N	-2.302501	-1.231567	0.453157
N	1.314807	1.420467	-0.150534
N	2.460705	-0.429557	-0.885134
C	0.026501	-0.552975	-1.087165
O	-1.095883	0.381909	-0.823876
N	2.897124	-1.578000	-0.182479
O	2.053926	-2.314512	0.266239
O	4.099545	-1.751795	-0.161052
N	0.818588	1.762146	1.115991
O	-0.041135	1.052393	1.595950
O	1.244953	2.793896	1.594316
C	-3.612912	1.532898	-1.405463
H	-4.655187	1.530935	-1.732732
H	-3.403635	2.437095	-0.824062
H	-2.949169	1.497332	-2.273150
C	-1.229299	-2.039485	1.049924
H	-0.447563	-1.371261	1.414911
H	-1.678148	-2.590221	1.881332
H	-0.803541	-2.713525	0.305640
C	-2.163679	-0.160911	-0.348528
C	1.132852	0.076198	-0.652399

8. $1NO_2 – CO – 1NH_2$

Charge = 0 Multiplicity = 1

C	-3.477101	-1.398885	0.858215
C	-4.235132	-0.472851	0.225114
H	-3.723570	-2.189582	1.552301
H	-5.295596	-0.266514	0.233000
C	2.647332	1.784014	-0.327590
C	3.341207	0.711373	-0.716135
H	2.976341	2.800562	-0.158031
H	4.395386	0.617033	-0.939830
N	-3.367472	0.278847	-0.554281
N	-2.158661	-1.200486	0.469559
N	1.268345	1.431813	-0.186911
N	2.467648	-0.406337	-0.863470
C	0.053562	-0.548263	-1.203439
O	-1.102263	0.367835	-0.995232
N	-3.754188	1.328299	-1.383214
N	-1.101730	-1.941608	1.020266
N	2.861287	-1.549333	-0.123379
O	1.991312	-2.278105	0.289330
O	4.057577	-1.725123	-0.032735
N	0.701885	1.753686	1.053910
O	-0.179374	1.030475	1.479054
O	1.091340	2.779631	1.568918
H	-3.275248	2.172613	-1.073674
H	-3.434889	1.120487	-2.328271
H	-0.545611	-1.289082	1.574871
H	-0.497605	-2.220809	0.242299
C	-2.104869	-0.168702	-0.393663
C	1.127043	0.092218	-0.709954

9. 1CHO – CO – 1CH_3

Charge = 0 Multiplicity = 1

C	-3.428252	-1.249930	0.767780
C	-4.014026	-0.301300	0.001715
H	-3.852903	-1.945979	1.477348
H	-5.048706	-0.004062	-0.094828
C	1.417020	0.055105	-0.262111
C	2.713222	1.848643	0.429674
C	3.552979	0.858814	0.105417
H	2.924935	2.862950	0.743429
H	4.634044	0.833523	0.065695
N	-3.006947	0.290947	-0.742021
N	-2.063688	-1.238042	0.499270
N	1.376177	1.364005	0.349135
N	2.813555	-0.283955	-0.218224
C	-1.826908	-0.274644	-0.412955
C	0.484738	-0.696932	-0.876834
O	-0.740131	0.137935	-0.952719
C	0.397353	1.842129	1.168255
O	-0.656714	1.292216	1.444367
H	0.664857	2.833868	1.579754
C	3.367630	-1.486019	-0.567325
O	4.568027	-1.679140	-0.601008
H	2.604399	-2.242923	-0.810923
C	-3.110665	1.417630	-1.651806

H	-2.677444	2.310904	-1.188393
H	-2.568671	1.189124	-2.573705
H	-4.167660	1.584278	-1.871314
C	-1.079048	-1.990070	1.282151
H	-0.424417	-2.550310	0.615156
H	-0.491191	-1.287571	1.878847
H	-1.644634	-2.663128	1.932907

10. 1CHO – CO – 1NH_2

Charge = 0 Multiplicity = 1

C	3.733857	-1.420442	0.319591
C	4.088158	-0.111859	0.334859
H	4.280697	-2.323179	0.551526
H	5.012552	0.390154	0.581443
C	-3.102790	1.607107	-0.435799
C	-3.714292	0.432131	-0.255427
H	-3.518850	2.578344	-0.670961
H	-4.761201	0.163629	-0.309252
N	2.966357	0.610008	-0.035253
N	2.406829	-1.483812	-0.076742
N	-1.704639	1.440013	-0.212272
N	-2.756946	-0.537991	0.062269
C	-0.340272	-0.718903	-0.256194
O	0.769781	0.177105	-0.621655
N	2.898765	2.003345	-0.067369
N	1.691265	-2.684856	-0.220575
O	-4.191904	-2.264097	0.422402
O	0.145506	2.372276	0.809403
H	2.816421	2.287958	-1.042210
H	2.023896	2.272884	0.396903
H	1.795296	-2.967126	-1.196406
H	0.696163	-2.371676	-0.122213
C	-0.945511	2.461771	0.271441
C	-3.056569	-1.831546	0.397295
H	-1.442956	3.437813	0.120018
H	-2.158644	-2.422779	0.638376
C	-1.446297	0.025729	-0.098103
C	1.943409	-0.236529	-0.274135

11. 1COOH – CO – 1CH_3

Charge = 0 Multiplicity = 1

C	-3.524374	-1.407110	-0.910482
C	-4.191727	-0.626393	-0.029328
H	-3.887426	-2.038321	-1.709255
H	-5.248924	-0.441546	0.099152
C	1.212158	0.026962	0.376705
C	2.404357	2.010057	0.194244
C	3.293195	1.024716	0.353877
H	2.549318	3.079827	0.152626
H	4.366991	1.058712	0.479771
N	-3.239553	-0.052265	0.796816
N	-2.166593	-1.308084	-0.632647
N	1.110879	1.430394	0.039998
N	2.630397	-0.214151	0.319509
C	-2.012778	-0.459220	0.403409
C	0.295765	-0.834278	0.859266

O	-0.959717	-0.029908	0.992683
C	-3.451339	0.912057	1.861042
H	-2.715586	0.729840	2.648368
H	-3.329229	1.932436	1.480538
H	-4.461104	0.777647	2.256607
C	-1.119164	-1.875507	-1.489847
H	-0.610911	-1.058826	-2.008825
H	-0.403327	-2.428394	-0.881130
H	-1.623328	-2.531010	-2.206021
C	0.165708	1.945153	-0.793708
O	-0.774025	1.354605	-1.296922
O	0.377558	3.270039	-1.008479
H	-0.323256	3.547838	-1.611761
C	3.328615	-1.380844	0.200457
O	4.542900	-1.446711	0.246615
O	2.537448	-2.451984	0.007831
H	3.145062	-3.201348	-0.053422

12. 1COOH – CO – 1NH_2

Charge = 0 Multiplicity = 1

C	-3.873000	-1.570164	0.320277
C	-4.268665	-0.273518	0.338841
H	-4.385028	-2.487664	0.572779
H	-5.200734	0.200494	0.610743
C	2.790698	1.655788	-0.546371
C	3.459368	0.507671	-0.415960
H	3.144840	2.646853	-0.788161
H	4.513514	0.290813	-0.524101
N	-3.181201	0.478990	-0.071015
N	-2.557503	-1.597243	-0.116902
N	1.412074	1.409875	-0.268314
N	2.566726	-0.520415	-0.072746
C	0.136756	-0.783978	-0.393493
O	-0.991855	0.113993	-0.721111
N	-3.144771	1.873397	-0.096528
N	-1.804122	-2.777946	-0.254848
H	-2.279549	2.153294	0.378879
H	-3.063433	2.164454	-1.069401
H	-0.813344	-2.413968	-0.203131
H	-1.928470	-3.082345	-1.221793
C	0.624667	2.331810	0.350385
O	-0.412004	2.131915	0.959367
O	1.134660	3.580621	0.199034
H	0.538843	4.166447	0.683193
C	3.032365	-1.760943	0.266285
O	4.211682	-2.058369	0.251959
O	2.058476	-2.613904	0.626194
H	2.517625	-3.430049	0.868065
C	1.222412	-0.020774	-0.195046
C	-2.139662	-0.337388	-0.336275

13. 2H – CO – 2H

Charge = -2 Multiplicity = 1

C	-3.901021	-0.788560	0.017339
C	-4.071307	0.556857	-0.003993
H	-4.658628	-1.563689	0.028826

H	-4.994550	1.124022	-0.009956
C	3.838544	0.919705	0.016692
C	4.164098	-0.404284	-0.014796
H	4.503269	1.776122	0.035336
H	5.149189	-0.857014	-0.033530
N	-2.814573	1.174095	-0.022340
H	-2.715968	2.177176	-0.042339
N	-2.534512	-1.073155	0.015371
H	-2.139078	-2.000632	0.014188
N	2.458663	1.038562	0.027575
H	1.998848	1.936577	0.049617
N	2.996111	-1.146936	-0.017302
H	3.002160	-2.155269	-0.046226
C	0.356550	-0.732116	0.028633
O	-0.426550	0.360935	-0.024676
B	1.856691	-0.269328	-0.012645
B	-1.815460	0.152858	-0.004333

14. $2CH_3 – CO – 2CH_3$

Charge = -2 Multiplicity = 1

C	3.942222	0.921203	-0.021008
C	4.098928	-0.426193	-0.001858
H	4.705783	1.691557	-0.037125
H	5.015607	-1.005360	-0.002555
C	-3.841129	-1.108533	-0.053250
C	-4.191407	0.211936	-0.040552
H	-4.489873	-1.978150	-0.081808
H	-5.186393	0.645081	-0.051259
N	2.843181	-1.028045	0.024563
N	2.584423	1.244053	-0.011531
N	-2.465236	-1.217111	-0.028370
N	-3.047822	0.980302	-0.012286
C	-0.436735	0.686603	-0.003388
O	0.485942	-0.295549	0.028690
B	-1.891788	0.111297	0.020007
B	1.856083	0.010516	0.006827
C	2.664364	-2.462749	0.008598
H	3.171531	-2.934506	0.860747
H	1.595161	-2.687198	0.072528
H	3.059544	-2.903031	-0.918901
C	2.154977	2.631242	-0.033598
H	1.063162	2.648386	-0.014217
H	2.553426	3.168095	0.838391
H	2.519437	3.128938	-0.945595
C	-1.803683	-2.504952	0.026418
H	-0.725453	-2.338308	0.037071
H	-2.089196	-3.053022	0.937524
H	-2.065158	-3.119653	-0.844190
C	-3.084068	2.425112	0.069029
H	-3.542827	2.752725	1.014572
H	-2.054872	2.794256	0.025646
H	-3.661533	2.849109	-0.763494

15. $2NH_2 – CO – 2NH_2$

Charge = -2 Multiplicity = 1

C	-4.141257	-0.264406	-0.119873

C	-3.862628	1.060401	0.015613
H	-5.092029	-0.775561	-0.209979
H	-4.539326	1.906004	0.058652
C	4.189896	0.136955	-0.146032
C	3.802473	-1.169193	0.007191
H	5.185983	0.553460	-0.246816
H	4.409339	-2.066332	0.059035
N	-2.489154	1.232928	0.127599
N	-2.938062	-0.969771	-0.104891
N	3.064268	0.924819	-0.207634
N	2.424644	-1.223943	0.041906
C	0.434845	0.675871	-0.079413
O	-0.511893	-0.391296	0.020546
B	1.849972	0.124152	-0.029389
B	-1.833383	-0.042133	0.017503
N	-1.910161	2.522064	0.251075
H	-1.851820	2.710827	1.253364
H	-0.919150	2.332501	-0.006886
N	-2.925546	-2.361127	-0.313440
H	-2.323598	-2.552573	-1.114878
H	-2.469306	-2.794633	0.486863
N	3.165769	2.328569	-0.219161
H	2.327829	2.638265	-0.714347
H	3.001977	2.644289	0.745386
N	1.784871	-2.423970	0.424431
H	1.673361	-2.389562	1.447395
H	0.832555	-2.331155	0.073167

16. 2CHO – CO – 2CHO

Charge = -2 Multiplicity = 1

C	-2.148832	-3.647381	0.000000
C	-3.024119	-2.623312	0.000000
H	-2.353617	-4.712388	0.000000
H	-4.107797	-2.657186	0.000000
N	-0.831402	-3.180130	0.000000
N	-2.353525	-1.386867	0.000000
O	0.162621	-5.255828	0.000000
O	-4.279554	-0.126932	0.000000
C	0.219502	-4.015412	0.000000
H	1.175995	-3.463618	0.000000
H	-2.376446	0.647689	0.000000
C	-3.041159	-0.231372	0.000000
C	1.986604	3.695392	0.000000
C	2.970571	2.776327	0.000000
H	2.046771	4.776540	0.000000
H	4.044055	2.922593	0.000000
N	0.737364	3.045491	0.000000
N	2.444836	1.473866	0.000000
O	-0.570309	4.929547	0.000000
O	4.496898	0.467850	0.000000
C	-0.445349	3.708562	0.000000
H	-1.308899	3.019609	0.000000
H	2.668642	-0.566560	0.000000
C	3.273317	0.362792	0.000000
C	0.384809	-0.813283	0.000000

O	0.000000	0.667747	0.000000
B	0.960256	1.554833	0.000000
B	-0.820039	-1.628063	0.000000

17. $2NO_2 – CO – 2NO_2$

Charge = -2 Multiplicity = 1

C	3.201037	0.939080	-1.561850
C	3.989030	0.171186	-0.791984
H	3.476961	1.654015	-2.323790
H	5.065528	0.088303	-0.775955
C	-3.232900	1.179730	1.118473
C	-3.976965	0.336358	0.383352
H	-3.540118	2.065642	1.655685
H	-5.038123	0.367328	0.184357
N	3.195229	-0.596059	0.075205
N	1.853847	0.717136	-1.245788
N	-1.898720	0.767210	1.122190
N	-3.183108	-0.678122	-0.154964
C	-0.581219	-1.300372	-0.234061
O	0.731478	-1.079998	0.222393
B	-1.687192	-0.507957	0.246836
B	1.716391	-0.347197	-0.183400
N	3.779014	-1.451891	0.932564
O	5.019308	-1.528925	0.913734
O	3.057249	-2.095304	1.673973
N	0.926009	1.620886	-1.679865
O	-0.133279	1.662801	-1.101557
O	1.251725	2.333792	-2.639301
N	-3.778696	-1.625061	-0.875579
O	-3.087784	-2.514060	-1.355840
O	-5.028081	-1.560446	-1.026362
N	-1.016773	1.479378	1.811333
O	0.149959	1.092090	1.844967
O	-1.415796	2.503830	2.413402

18. $2NO_2 – CO – 2CH_3$

Charge = -2 Multiplicity = 1

C	-4.404099	-1.328360	-0.029369
C	-4.707966	-0.001286	-0.096885
H	-5.086549	-2.173175	0.005845
H	-5.687672	0.467608	-0.127181
C	3.251204	1.338552	-0.301271
C	3.693329	0.069566	-0.284229
H	3.810475	2.249597	-0.459195
H	4.696709	-0.300634	-0.436358
N	-3.527785	0.728586	-0.122404
N	-3.025633	-1.503963	-0.007947
N	1.875520	1.376051	-0.047430
N	2.644499	-0.813639	-0.023325
C	-0.042856	-0.689993	0.056980
O	-1.126535	0.253983	-0.098298
N	2.931596	-2.108301	0.061513
O	2.022829	-2.895000	0.314752
O	4.129390	-2.473410	-0.128547
N	1.325184	2.561765	0.187841
O	0.167576	2.606784	0.606848

O	2.016534	3.596953	-0.026372
C	-3.449018	2.164139	-0.154239
H	-4.005811	2.619095	0.683035
H	-2.390526	2.440399	-0.065810
H	-3.848428	2.579322	-1.096315
C	-2.412373	-2.814710	0.067044
H	-1.322805	-2.647987	0.102826
H	-2.746151	-3.349671	0.973593
H	-2.678059	-3.423167	-0.815300
B	-2.392432	-0.191356	-0.069816
B	1.281924	-0.066005	0.070191

19. $2NO_2 – CO – 2NH_2$

Charge = -2 Multiplicity = 1

C	-4.228332	-1.473121	0.255601
C	-4.584710	-0.156859	0.194782
H	-4.836674	-2.338197	0.498061
H	-5.547301	0.310696	0.370561
C	3.011397	1.553265	-0.290993
C	3.623241	0.357676	-0.223446
H	3.448609	2.530605	-0.440214
H	4.672879	0.124976	-0.332638
N	-3.465520	0.582815	-0.182350
N	-2.887239	-1.604716	-0.073598
N	1.631904	1.402392	-0.090201
N	2.693178	-0.654819	0.024979
C	-0.014390	-0.818830	-0.158078
O	-1.060618	0.118832	-0.554898
B	1.249759	-0.100917	0.006300
B	-2.316588	-0.297729	-0.308331
N	-3.437020	1.992197	-0.109551
N	-2.184434	-2.833096	0.033232
N	3.127756	-1.904429	0.130679
O	2.303154	-2.783851	0.366771
O	4.360706	-2.130058	-0.025880
N	0.935211	2.490171	0.236568
O	-0.184908	2.357897	0.732216
O	1.460717	3.617137	0.027776
H	-2.577911	2.227010	0.397172
H	-3.254632	2.331859	-1.053531
H	-1.193428	-2.482142	0.161051
H	-2.149899	-3.217631	-0.913696

20. $2CHO – CO – 2CH_3$

Charge = -2 Multiplicity = 1

C	4.159280	-1.310914	-0.015319
C	4.436749	0.023538	-0.023988
H	4.858019	-2.143070	-0.020379
H	5.408861	0.509410	-0.033795
C	-3.530583	1.410970	-0.005673
C	-3.989011	0.146274	-0.011512
H	-4.127593	2.320513	-0.006897
H	-5.016563	-0.200141	-0.019553
N	3.245451	0.733494	-0.017319
N	2.781918	-1.510538	-0.001061
N	-2.125277	1.474038	0.005350

N	-2.928767	-0.758243	-0.005658
C	-0.281887	-0.681270	0.028339
O	0.856308	0.216024	0.020921
C	-1.555432	2.699525	0.000981
O	-0.364689	3.003877	0.010414
H	-2.328735	3.507720	-0.015276
C	-3.141145	-2.082915	-0.006329
O	-4.255635	-2.639389	-0.009906
H	-2.191166	-2.644148	-0.004085
C	3.137515	2.168676	0.001324
H	3.607950	2.625178	-0.886203
H	2.069349	2.422956	0.008667
H	3.614861	2.601547	0.898912
C	2.188760	-2.828479	0.019617
H	1.098049	-2.681508	0.031773
H	2.481794	-3.409693	-0.872346
H	2.504385	-3.390914	0.917680
B	2.124067	-0.206852	0.007439
B	-1.569233	0.005726	-0.000189

21. $2CHO – CO – 2NH_2$

Charge = -2 Multiplicity = 1

C	4.132845	-1.344640	0.001927
C	4.531293	-0.044310	-0.120989
H	4.736778	-2.246090	0.010333
H	5.524741	0.376111	-0.229191
C	-3.425004	1.272689	0.030596
C	-3.867540	0.001618	-0.038358
H	-4.004990	2.188689	0.063407
H	-4.891053	-0.356104	-0.073783
N	3.392926	0.760494	-0.081962
N	2.757085	-1.399661	0.129941
N	-2.021406	1.321006	0.055944
N	-2.801607	-0.902995	-0.064416
C	-0.123522	-0.700882	-0.009968
O	0.931745	0.384655	0.057214
B	-1.453351	-0.127911	-0.000565
B	2.192332	-0.067185	0.046001
N	3.470887	2.151679	-0.280734
N	2.034566	-2.620360	0.220537
O	-4.105002	-2.798909	-0.180417
O	-1.913070	3.619504	0.170597
H	2.879895	2.368511	-1.084498
H	2.992134	2.589341	0.506307
H	1.040641	-2.244953	0.022331
H	1.975045	-2.826457	1.222227
C	-1.373192	2.496304	0.122541
C	-3.001284	-2.225820	-0.133430
H	-0.279209	2.365481	0.132226
H	-2.047012	-2.781948	-0.144767

22. $2COOH – CO – 2CH_3$

Charge = -2 Multiplicity = 1

C	4.348173	-1.442412	-0.041249
C	4.702656	-0.130041	-0.144891
H	5.000076	-2.311170	0.000220

H	5.699588	0.298703	-0.203059
N	3.549911	0.643632	-0.173673
N	2.966320	-1.566262	0.001669
C	-0.012215	-0.684254	0.001579
O	1.127706	0.250261	-0.090241
B	2.370609	-0.231325	-0.082272
C	-3.195651	1.422860	-0.446905
C	-3.677845	0.169892	-0.446462
H	-3.722416	2.343500	-0.672043
H	-4.683455	-0.159435	-0.681347
N	-2.701018	-0.762542	-0.073667
N	-1.845512	1.453534	-0.057679
B	-1.308016	-0.032551	0.040888
C	-1.324751	2.651008	0.225690
O	-1.869938	3.758923	0.052993
O	-0.081354	2.610134	0.780680
H	0.120171	3.541591	0.925080
C	-3.090320	-2.035720	0.055744
O	-4.237622	-2.483203	-0.145019
O	-2.108773	-2.884629	0.454524
H	-2.562088	-3.734734	0.501542
C	3.530199	2.075425	-0.248659
H	2.479134	2.386857	-0.204706
H	4.074811	2.541331	0.592953
H	3.973269	2.450785	-1.188973
C	2.303378	-2.849132	0.114037
H	2.607733	-3.368755	1.041068
H	1.219547	-2.629478	0.130440
H	2.550854	-3.495983	-0.747597

23. $2COOH – CO – 2NH_2$

Charge = -2 Multiplicity = 1

C	-4.120782	-1.688231	0.005352
C	-4.699004	-0.467426	-0.140298
H	-4.579676	-2.666321	0.020275
H	-5.739035	-0.198047	-0.258761
C	3.234790	1.467165	-0.061393
C	3.702976	0.215330	-0.130140
H	3.799859	2.386938	-0.068622
H	4.730708	-0.099547	-0.204359
N	-3.684126	0.501847	-0.099541
N	-2.761319	-1.550980	0.153887
N	1.843824	1.506361	0.027815
N	2.652776	-0.724202	-0.088198
C	-0.012903	-0.589499	-0.024113
O	-1.168917	0.417051	0.071395
B	1.286482	0.040319	-0.012803
B	-2.381968	-0.149567	0.050111
N	-3.926580	1.859369	-0.327879
N	-1.900888	-2.680486	0.261113
H	-4.346313	1.981364	-1.246898
H	-4.581281	2.209032	0.367328
H	-1.786790	-2.837768	1.264328
H	-0.958553	-2.205142	0.014912
C	1.252297	2.732107	0.129531

O	1.882279	3.790061	0.156477
O	-0.075611	2.753943	0.203166
H	-0.514517	1.856950	0.148707
C	2.889292	-2.034408	-0.075019
O	2.115205	-2.971670	-0.011942
O	4.265025	-2.336398	-0.145022
H	4.263368	-3.298721	-0.129939

24. 1H – CO – 2H

Charge = -1 Multiplicity = 1

C	-3.750933	-0.853707	0.144172
C	-4.003642	0.480457	0.101204
H	-4.468634	-1.661968	0.231232
H	-4.962494	0.984490	0.145723
C	1.746991	-0.314079	-0.248111
C	3.566012	0.941788	0.288563
C	3.947963	-0.348197	0.321103
H	4.159050	1.823807	0.510556
H	4.922825	-0.755428	0.569305
N	-2.789509	1.169686	-0.009477
N	-2.378835	-1.060185	0.060536
N	2.277204	1.034322	-0.283643
N	2.925510	-1.155298	-0.228214
C	0.474751	-0.733789	-0.144263
O	-0.375352	0.468294	-0.144909
H	2.737973	-2.033300	0.242680
H	1.624136	1.689890	0.132451
H	-1.902946	-1.949033	0.065693
H	-2.751998	2.172056	-0.071765
B	-1.696508	0.205724	-0.043402

25. $1CH_3 – CO – 2CH_3$

Charge = -1 Multiplicity = 1

C	3.812351	-1.002742	-0.094675
C	4.046889	0.332690	-0.015310
H	4.534161	-1.809062	-0.179939
H	4.997164	0.857197	-0.018712
C	-1.802111	-0.105464	0.223400
C	-3.688961	1.171797	-0.001700
C	-4.080478	-0.115657	0.042506
H	-4.298864	2.065933	-0.083144
H	-5.084877	-0.524311	-0.007368
N	2.828871	0.998948	0.073971
N	2.442745	-1.252644	-0.057110
N	-2.301837	1.262213	0.242827
N	-2.987796	-0.923495	0.335612
C	-0.566814	-0.647160	0.126899
O	0.449334	0.389428	0.132209
B	1.749098	0.019892	0.055121
C	2.715481	2.426971	0.191279
H	3.189710	2.944094	-0.658427
H	1.650792	2.682204	0.205110
H	3.173956	2.801271	1.121424
C	1.932466	-2.606393	-0.137104
H	2.316880	-3.215515	0.697521
H	0.839648	-2.544604	-0.083041

H	2.239030	-3.081107	-1.083685
C	-1.594311	2.233945	-0.573782
H	-0.615924	2.449301	-0.141078
H	-1.444910	1.854386	-1.602174
H	-2.192742	3.154902	-0.609966
C	-2.916500	-2.280219	-0.140992
H	-2.624904	-2.318315	-1.207760
H	-2.146263	-2.813882	0.425578
H	-3.894978	-2.759134	0.002159

26. $1NH_2 – CO – 2NH_2$

Charge = -1 Multiplicity = 1

C	-4.068209	-0.221428	-0.123295
C	-3.749587	1.090359	0.035859
H	-5.034045	-0.698090	-0.237614
H	-4.397520	1.957838	0.079978
C	4.054955	0.110244	-0.178331
C	3.676512	-1.166947	0.002743
H	5.047870	0.543672	-0.215766
H	4.277495	-2.056134	0.154973
N	-2.369554	1.219791	0.145129
N	-2.885563	-0.961503	-0.130286
N	2.939890	0.890860	-0.500724
N	2.276445	-1.285724	-0.152246
C	0.528946	0.584596	-0.151011
O	-0.451642	-0.479359	0.001654
B	-1.749119	-0.073858	0.014021
N	-1.865228	-1.534305	0.482827
N	-1.764865	2.492421	0.295032
H	-1.662763	2.644736	1.300683
H	-0.794251	2.310337	-0.017646
N	-2.903952	-2.347466	-0.367319
H	-2.311899	-2.528873	-1.177013
H	-2.442360	-2.803886	0.417433
N	2.925081	2.213025	-0.003833
H	2.269070	2.708912	-0.605942
H	2.426764	2.171670	0.896171
N	1.690430	-2.095854	0.866893
H	1.591222	-1.491704	1.693721
H	0.732545	-2.244237	0.557429
C	1.774253	0.071688	-0.252341

27. 1COOH – CO – 2COOH

Charge = -1 Multiplicity = 1

C	3.472221	1.918425	-0.021549
C	4.016282	0.718887	-0.275349
H	3.940541	2.894833	-0.008708
H	5.040435	0.472955	-0.516903
C	-1.726954	-0.227322	-0.128510
C	-3.087887	-1.571039	1.168360
C	-3.833271	-0.524823	0.784396
H	-3.318330	-2.384939	1.843332
H	-4.838895	-0.250048	1.067244
N	3.016840	-0.283215	-0.180406
N	2.109149	1.782195	0.288360
N	-3.100599	0.241567	-0.154087

C	-0.647253	0.566567	-0.281694
O	0.529248	-0.216843	0.080081
B	1.708148	0.380881	0.106720
C	-3.637358	1.167873	-0.978677
O	-3.109086	1.765281	-1.891639
O	-4.959875	1.402380	-0.652204
H	-5.229748	2.072447	-1.291159
C	-1.067444	-2.635896	0.345429
O	-1.090029	-3.576841	1.124360
O	-0.312414	-2.587252	-0.764988
H	0.597915	-2.846412	-0.543773
C	1.380249	2.887233	0.696166
O	1.658925	4.030193	0.404362
O	0.397357	2.541650	1.534624
H	-0.241407	3.265754	1.542218
C	3.255869	-1.602040	-0.418197
O	2.462584	-2.518329	-0.338878
O	4.553232	-1.836350	-0.761401
H	4.601368	-2.790977	-0.899489

28. 1CHO – CO – 2CHO

Charge = -1 Multiplicity = 1

C	-3.671524	1.364120	-0.071104
C	-4.000502	0.060949	-0.082896
H	-4.307416	2.240075	-0.070120
H	-4.975867	-0.409154	-0.089073
C	1.838036	-0.092750	0.034835
C	3.484350	-1.557192	-0.677374
C	4.068777	-0.360096	-0.536078
H	3.900712	-2.485388	-1.050156
H	5.076165	-0.034607	-0.758864
N	-2.828430	-0.719512	-0.073800
N	-2.265354	1.516280	-0.056183
N	2.152255	-1.492675	-0.204185
N	3.143741	0.531419	0.017840
C	0.688497	0.607569	0.030084
O	-0.412677	-0.285745	-0.115402
B	-1.663375	0.175777	-0.071799
C	3.450447	1.784992	0.435975
O	4.559998	2.291042	0.307692
H	2.584883	2.291435	0.892189
C	1.499074	-2.614321	0.213560
O	0.486669	-2.685252	0.883137
H	2.025247	-3.523988	-0.147691
C	-2.819675	-2.093252	-0.008082
O	-3.827552	-2.775729	-0.018890
H	-1.796632	-2.503036	0.068683
C	-1.678362	2.771664	-0.047062
O	-2.329154	3.799953	-0.055915
H	-0.578691	2.712945	-0.027797

29. $1NO_2 – CO – 2NO_2$

Charge = -1 Multiplicity = 1

C	-3.216479	1.598150	0.468742
C	-3.829531	0.433820	0.214196
H	-3.597727	2.486698	0.950213

H	-4.842554	0.123808	0.423654
C	1.622673	-0.415078	-0.567043
C	2.592977	-2.088452	0.722404
C	3.563361	-1.553159	-0.025699
H	2.611615	-2.956515	1.366599
H	4.592443	-1.864235	-0.139482
N	-2.923297	-0.427085	-0.429815
N	-1.896634	1.554308	-0.013663
N	1.397006	-1.349260	0.529292
N	3.056966	-0.445996	-0.753377
C	0.764878	0.056199	-1.496082
O	-0.550561	-0.361482	-1.147810
B	-1.580163	0.218182	-0.591283
N	0.684485	-1.028032	1.660119
O	0.814008	-1.775053	2.622123
O	-0.079438	-0.081438	1.604998
N	3.833034	0.717673	-0.675510
O	3.286799	1.775238	-0.848624
O	5.037043	0.540228	-0.520529
N	-3.299667	-1.694532	-0.766879
O	-4.447955	-2.022529	-0.495507
O	-2.474692	-2.393892	-1.311671
N	-1.034154	2.586870	0.283335
O	-1.493097	3.506442	0.946691
O	0.086094	2.504088	-0.146944

30. $1NO_2 – CO – 2CH_3$

Charge = -1 Multiplicity = 1

C	-4.373208	-1.231544	0.077579
C	-4.591056	0.102355	-0.053200
H	-5.099502	-2.037615	0.092502
H	-5.532873	0.627585	-0.173018
C	1.208100	-0.198830	0.200466
C	2.783133	1.237237	1.129411
C	3.331009	0.016523	1.107151
H	3.153661	2.155249	1.565077
H	4.271622	-0.323850	1.516883
N	-3.368386	0.765385	-0.020562
N	-3.006331	-1.481883	0.198510
N	1.525503	1.193564	0.482437
N	2.458172	-0.885084	0.445135
C	-0.003881	-0.808587	0.211974
O	-1.004682	0.164342	0.231020
B	-2.320072	-0.213661	0.141681
N	1.234911	2.226212	-0.381496
O	1.735335	3.318691	-0.109758
O	0.458671	2.013369	-1.285605
N	3.057506	-1.706671	-0.503430
O	2.367677	-2.160707	-1.383764
O	4.240523	-1.980409	-0.305691
C	-3.223007	2.190951	-0.183363
H	-3.675819	2.743322	0.654613
H	-2.153532	2.422884	-0.225699
H	-3.690189	2.532802	-1.119051
C	-2.504877	-2.832678	0.356968

H	-1.412142	-2.787255	0.365490
H	-2.868920	-3.274234	1.297817
H	-2.839048	-3.466111	-0.478729

31. $1NO_2 – CO – 2NH_2$

Charge = -1 Multiplicity = 1

C	4.302540	-1.330914	-0.028322
C	4.642408	-0.021686	-0.160406
H	4.935647	-2.208199	0.028691
H	5.617029	0.445221	-0.230304
C	-1.177664	-0.137489	-0.245547
C	-2.780579	1.355162	-1.013013
C	-3.293276	0.127180	-1.148890
H	-3.171292	2.308329	-1.342561
H	-4.217239	-0.186674	-1.614235
N	3.470796	0.731724	-0.218366
N	2.916016	-1.444918	0.018930
N	-1.527206	1.268507	-0.357099
N	-2.401211	-0.825873	-0.592458
C	0.052321	-0.701862	-0.290763
O	1.030212	0.293049	-0.172001
B	2.329642	-0.142004	-0.119091
N	3.511698	2.130581	-0.361994
H	2.975039	2.369444	-1.194222
H	2.996189	2.534478	0.418760
N	2.300379	-2.712066	0.161731
H	2.155821	-2.854312	1.163193
H	1.348082	-2.556127	-0.195962
N	-1.311853	2.170707	0.671339
O	-0.567716	1.846600	1.566849
O	-1.841737	3.272973	0.540804
N	-2.984027	-1.776499	0.238956
O	-4.160274	-2.045398	0.005238
O	-2.283500	-2.327177	1.053668

32. $1CHO – CO – 2CH_3$

Charge = -1 Multiplicity = 1

C	-4.078445	-1.518942	0.146470
C	-4.420500	-0.209835	0.286584
H	-4.676396	-2.410678	0.293323
H	-5.362930	0.236156	0.580908
C	2.857630	1.525464	-0.679031
C	3.485252	0.346851	-0.578748
H	3.239057	2.484375	-1.000426
H	4.511675	0.079730	-0.790934
N	-3.310430	0.572607	-0.026586
N	-2.748772	-1.604445	-0.258187
N	1.518016	1.368587	-0.245002
N	2.590456	-0.619379	-0.091529
C	0.110799	-0.742605	-0.367460
O	-0.937671	0.176502	-0.619539
N	-3.295266	1.963448	0.202201
N	-2.102359	-2.855149	-0.400764
H	-2.421539	2.161655	0.695866
H	-3.192909	2.418895	-0.703802
H	-1.115477	-2.635297	-0.195776

H	-2.095452	-3.068470	-1.399302
C	0.798956	2.365014	0.322207
O	-0.191010	2.286212	1.024179
O	1.331802	3.594479	-0.000944
H	0.754657	4.220602	0.451692
C	3.040667	-1.819008	0.339794
O	4.208668	-2.189267	0.251404
O	2.083473	-2.591528	0.889869
H	2.547879	-3.394735	1.157120
C	1.249106	-0.060472	-0.132949
B	-2.194593	-0.280378	-0.346109

33. 1CHO – CO – $2NH_2$

Charge = -1 Multiplicity = 1

C	4.055581	-1.288067	0.042160
C	4.401823	0.015184	-0.124014
H	4.682455	-2.170811	0.081754
H	5.376738	0.470493	-0.246738
C	-3.349391	1.252106	0.141467
C	-3.776400	-0.014347	0.056647
H	-3.895978	2.179644	0.240789
H	-4.776317	-0.426677	0.064598
N	3.236471	0.781435	-0.129810
N	2.672337	-1.386020	0.161670
N	-1.942703	1.274924	0.070751
N	-2.672686	-0.864439	-0.072074
C	-0.217868	-0.639709	-0.026015
O	0.796289	0.365889	0.033853
B	2.088081	-0.079404	0.033380
N	3.287371	2.171093	-0.336508
N	2.049591	-2.646275	0.333724
O	-3.845043	-2.808754	-0.264358
O	-1.793928	3.543781	0.186642
H	2.715493	2.387119	-1.151664
H	2.829624	2.623238	0.452947
H	1.079669	-2.465799	0.035348
H	1.964103	-2.792208	1.341596
C	-1.248243	2.445556	0.091111
C	-2.775838	-2.204866	-0.243110
H	-0.163167	2.304710	0.016357
H	-1.791147	-2.684330	-0.356927
C	-1.445181	-0.090974	-0.019633

34. 1COOH – CO – $2CH_3$

Charge = -1 Multiplicity = 1

C	4.186270	-1.481846	-0.047159
C	4.526983	-0.176262	-0.201970
H	4.840161	-2.343883	0.038770
H	5.516862	0.263436	-0.269772
C	-1.293263	-0.025858	-0.029192
C	-2.785199	1.557150	-0.845963
C	-3.410657	0.373082	-0.886516
H	-3.099416	2.528995	-1.202106
H	-4.375020	0.100542	-1.293141
N	3.366044	0.586953	-0.275129
N	2.798491	-1.613873	-0.013569

N	-1.563254	1.403369	-0.155812
N	-2.617774	-0.592834	-0.237899
C	-0.138063	-0.713307	-0.146366
O	0.949154	0.189870	-0.196418
B	2.221698	-0.294712	-0.160366
C	3.355693	2.018598	-0.426646
H	3.849160	2.331319	-1.360215
H	2.311647	2.348163	-0.455159
H	3.860254	2.519183	0.414961
C	2.174460	-2.910956	0.157460
H	1.090006	-2.761276	0.169043
H	2.443285	-3.582520	-0.673104
H	2.502737	-3.374749	1.101100
C	-1.011640	2.454545	0.492750
O	-1.294588	3.629957	0.275582
O	-0.111787	2.103029	1.437377
H	0.206044	2.943754	1.788629
C	-3.133829	-1.790972	0.105908
O	-4.256822	-2.178449	-0.211159
O	-2.304839	-2.551186	0.853089
H	-2.812241	-3.355516	1.018088

35. 1COOH – CO – 2NH_2

Charge = -1 Multiplicity = 1

C	-4.078445	-1.518942	0.146470
C	-4.420500	-0.209835	0.286584
H	-4.676396	-2.410678	0.293323
H	-5.362930	0.236156	0.580908
C	2.857630	1.525464	-0.679031
C	3.485252	0.346851	-0.578748
H	3.239057	2.484375	-1.000426
H	4.511675	0.079730	-0.790934
N	-3.310430	0.572607	-0.026586
N	-2.748772	-1.604445	-0.258187
N	1.518016	1.368587	-0.245002
N	2.590456	-0.619379	-0.091529
C	0.110799	-0.742605	-0.367460
O	-0.937671	0.176502	-0.619539
N	-3.295266	1.963448	0.202201
N	-2.102359	-2.855149	-0.400764
H	-2.421539	2.161655	0.695866
H	-3.192909	2.418895	-0.703802
H	-1.115477	-2.635297	-0.195776
H	-2.095452	-3.068470	-1.399302
C	0.798956	2.365014	0.322207
O	-0.191010	2.286212	1.024179
O	1.331802	3.594479	-0.000944
H	0.754657	4.220602	0.451692
C	3.040667	-1.819008	0.339794
O	4.208668	-2.189267	0.251404
O	2.083473	-2.591528	0.889869
H	2.547879	-3.394735	1.157120
C	1.249106	-0.060472	-0.132949
B	-2.194593	-0.280378	-0.346109