Electronic Supplementary Information

for

Unveiling the Energetic Potential of Azahomocubane (AHC): A New Class of Potential Propellants, Explosives and Oxidizers

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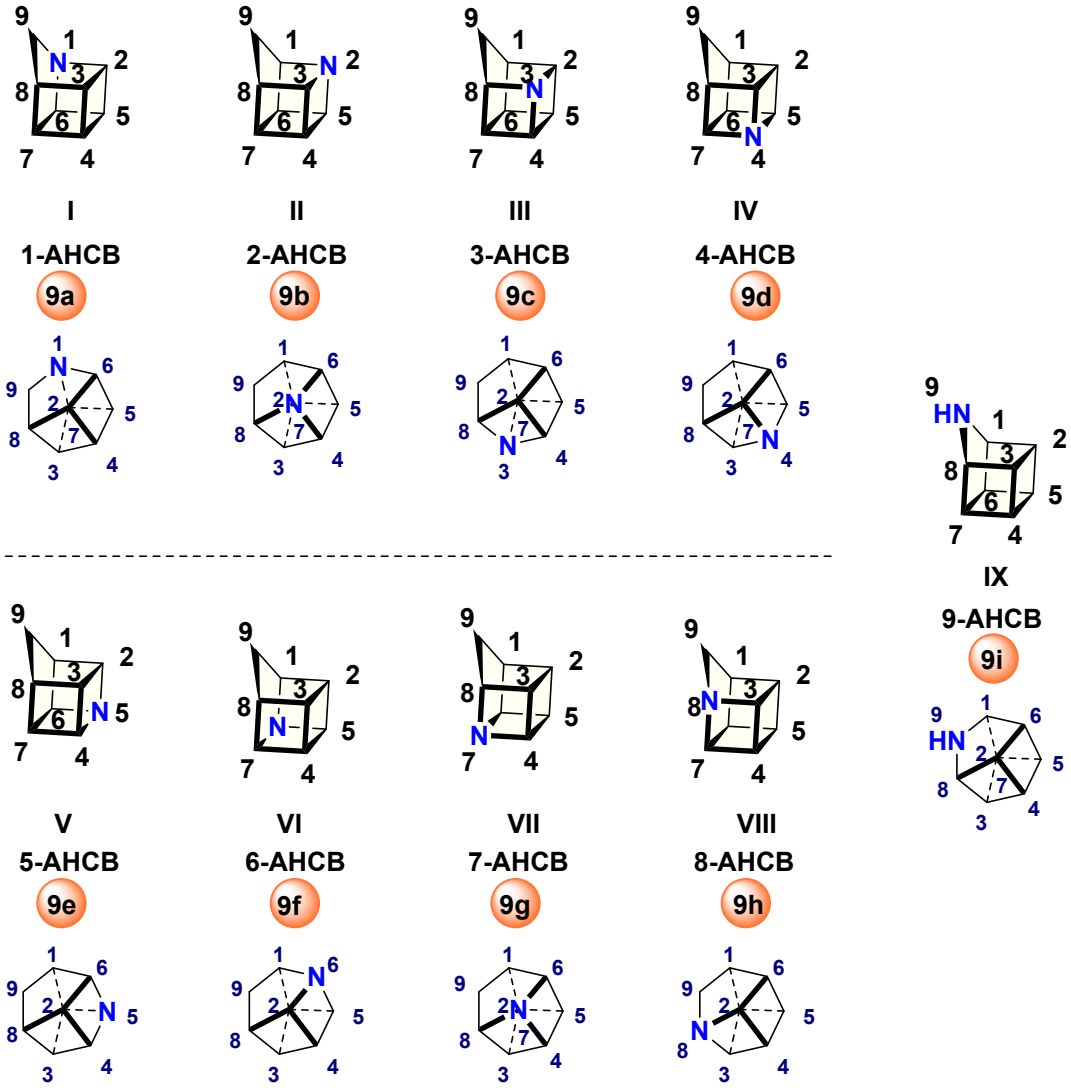


Figure S1. Possible isomers of azahomocubanes and their Schlegel diagrams.

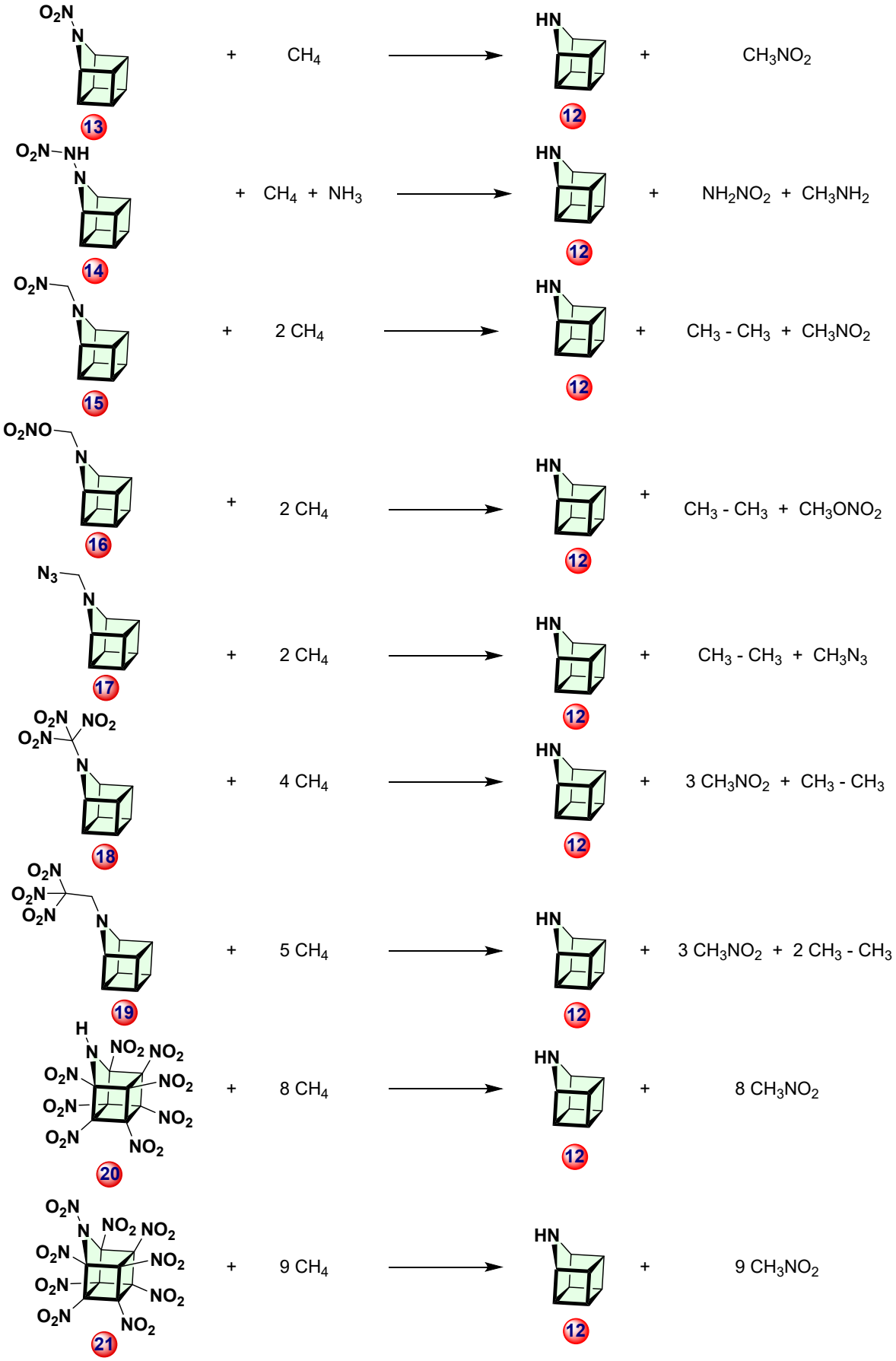
Table S1. Calculated Total Energy (E_0), Zero-point Energy (ZPE), values of Thermal Correction (H_T) and Enthalpy of Formation ($\Delta H_f°$ (g)) of the compounds using B3LYP/6-31+G**//MP2/6-311++G** level of theory (Isodesmic)[1]

Compound	E_0 [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	$\Delta H_f°$ (g) kJ/mol	$\Delta H_{sub}°$ (g) kJ/mol	$\Delta H_f°$ (s) kJ/mol	Density
AHC-12	0.005918	0.153015	0.158933	456.40	66.18	390.22	1.33
AHC-13	0.008408	0.155459	0.163867	456.70	54.34	402.36	1.53
AHC-14	0.009691	0.171605	0.181296	547.79	93.43	454.36	1.53
AHC-15	0.009201	0.183551	0.192752	447.30	91.28	356.02	1.47
AHC-16	0.01108	0.187383	0.198463	384.32	94.50	289.82	1.51
AHC-17	0.010064	0.184083	0.194147	818.14	89.73	728.41	1.40
AHC-18	0.015438	0.186342	0.20178	447.90	102.45	345.45	1.71
AHC-19	0.016424	0.21543	0.231854	438.50	116.05	322.45	1.66
AHC-20	0.028487	0.167456	0.195943	458.80	149.76	309.04	2.08
AHC-21	0.031094	0.168077	0.199171	459.10	154.16	304.94	2.14
CH_4	-40.3796224	0.044793	0.003812	-74.60[a]	----	----	----
NH_3	-56.43462	0.034377	0.003818	-45.9[a]	----	----	----
CH_3NO_2	-244.4784821	0.049840	0.005298	-74.30[a]	----	----	----
CH_3N_3	-203.60768	0.050250	0.005430	296.54	----	----	----
CH_3ONO_2	-319.509055	0.054251	0.005933	-137.28[b]	----	----	----
CH_3-CH_3	-79.5716305	0.07461	0.004428	-84.00[b]	----	----	----
NH_2-NO_2	-260.4931748	0.039257	0.004652	-6.11[b]	----	----	----
CH_3-NH_2	-95.5938424	0.064026	0.004375	-23.00[a]	----	----	----

[a] Data are from Ref. [D. R. Lide ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version **2008**), CRC Press/Taylor and Francis, Boca Raton, FL.]. [b]Obtained at G2 level.

The oxygen balance for $C_aH_bN_cO_d$ was calculated by using equation S1.

$$OB^{CO2}(\%) = -1600(2a-0.5b-d)/MW \quad \text{(S1)}$$



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igure S2. Isodesmic reactions for compounds **AHC-13-21**.

Table S2. The Gas phase heats of formation $\Delta H_f°(g)$ was predicted according to isodesmic equations S2-S10.

For compound AHC-13

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + \Delta H_f°(g)_{CH3\text{-}NO2} - \Delta H_f°(g)_{CH4} \quad (S2)$$

For compound AHC-14

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + \Delta H_f°(g)_{NH2\text{-}NO2} + \Delta H_f°(g)_{CH3\text{-}NH2} - \Delta H_f°(g)_{CH4} - \Delta H_f°(g)_{NH3} \quad (S3)$$

For compound AHC-15

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + \Delta H_f°(g)_{CH3\text{-}CH3} + \Delta H_f°(g)_{CH3\text{-}NO2} - 2\,\Delta H_f°(g)_{CH4} \quad (S4)$$

For compound AHC-16

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + \Delta H_f°(g)_{CH3\text{-}CH3} + \Delta H_f°(g)_{CH3\text{-}ONO2} - 2\,\Delta H_f°(g)_{CH4} \quad (S5)$$

For compound AHC-17

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + \Delta H_f°(g)_{CH3\text{-}CH3} + \Delta H_f°(g)_{CH3\text{-}N3} - 2\,\Delta H_f°(g)_{CH4} \quad (S6)$$

For compound AHC-18

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + \Delta H_f°(g)_{CH3\text{-}CH3} + 3\,\Delta H_f°(g)_{CH3\text{-}NO2} - 4\,\Delta H_f°(g)_{CH4} \quad (S7)$$

For compound AHC-19

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + 2\,\Delta H_f°(g)_{CH3\text{-}CH3} + 3\,\Delta H_f°(g)_{CH3\text{-}NO2} - 5\,\Delta H_f°(g)_{CH4} \quad (S8)$$

For compound AHC-20

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + 8\,\Delta H_f°(g)_{CH3\text{-}NO2} - 8\,\Delta H_f°(g)_{CH4} \quad (S9)$$

For compound AHC-21

$$\Delta H_f°(g)_{\mathbf{Compd13}} = \Delta H_f°(g)_{\mathbf{Compd12}} + 9\,\Delta H_f°(g)_{CH3\text{-}NO2} - 9\,\Delta H_f°(g)_{CH4} \quad (S10)$$

Subsequently, their solid phase enthalpies of formation $\Delta H_f°$ (s) were calculated by using equations S11-S12.[2-4]

$$\Delta H_f° (s) = \Delta H_f° (g) - \Delta H_{sub} \quad (S11)$$

Where, $\Delta Hf°(s)$ is solid phase enthalpy of formation, $\Delta H_f°(g)$ is enthalpy of formation in gas phase and ΔH_{sub} is represent the enthalpy of sublimation.

$$\Delta H_{sub} = a(SA)^2 + b\sqrt{(\sigma^2_{tot}\upsilon)} + c \quad (S12)$$

Where, *a*, *b* and *c* are fitting parameters, SA is the surface area of the 0.001 electron bohr^{-3} isosurface of the electrostatic potential of the molecules, σ^2_{tot} is the measure of variability of electronic potential on the surface, and υ is the degree of balance between the positive and negative charges on the isosurface.

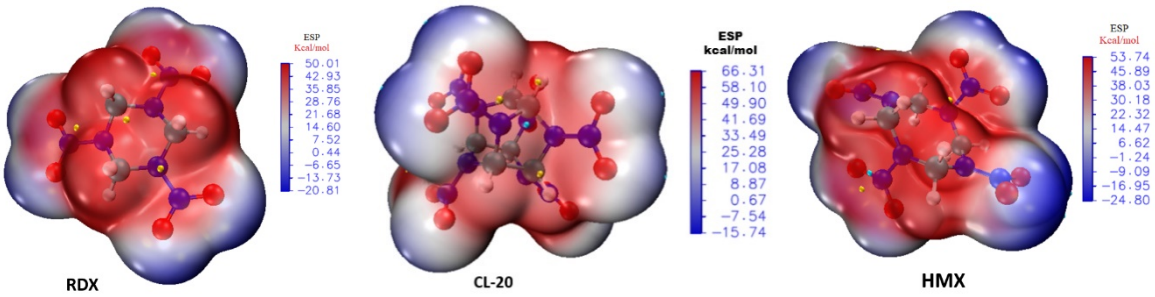


Figure S3. Computed electrostatic potential (ESP) maps of (a) RDX, (b) CL-20 and (c) HMX.

Impact sensitivity

The impact sensitivity (h_{50}) of the title compounds were predicted by using equation S13.[5]

$$h_{50\,[cm]} = \alpha\sigma^2_{+} + \beta\upsilon + \gamma \qquad \text{(S13)}$$

Where, the coefficients α, β, γ are -0.0064, 241.42 and -3.43, respectively. The σ^2_{+} is the measure of variability of the positive surface potentials and υ is the degree of balance between the positive and negative charges on the isosurface.

Then their corresponding impact energies were calculated by using 2.5 kg hammer weight.

Table S3. Total surface area (SA), σ^2_{tot}, σ^2_{+}, balance of charges, impact sensitivity ($h_{50[cm]}$) and impact energy [$h_{50[J]}$].

Compound	SA[a] Å^2	σ^2_{tot}[b] (kcal/mol)^2	σ^2_{+}[c] (kcal/mol)^2	υ[d]	h_{50}[e] [cm]	h_{50}[f] [J]
CL-20	324.62	239.42	224.49	0.05844748	9.25	2.27 (2.9)*
RDX	209.49	214.34	182.25	0.12731604	26.14	6.41 (7.5)*
HMX	251.50	246.97	207.61	0.13397103	27.58	6.76 (7.5)*
ONC	329.41	161.92	156.86	0.03025322	2.86	0.70 (<1)*
AHC-12	153.44	124.77	18.59	0.12683024	27.07	6.64
AHC-13	179.37	116.11	13.93	0.10555878	21.96	5.38
AHC-14	198.35	28.80	39.83	0.20025032	44.66	10.95
AHC-15	201.13	124.40	32.01	0.19109977	42.50	10.42
AHC-16	215.97	93.10	26.24	0.20239347	45.26	11.10
AHC-17	207.12	97.96	23.96	0.18476406	41.02	10.06
AHC-18	239.90	55.58	27.01	0.24980483	56.70	13.90
AHC-19	261.01	69.77	45.33	0.22757894	51.22	12.56
AHC-20	325.10	164.69	156.52	0.04719538	6.96	1.71
AHC-21	335.13	119.93	114.12	0.04613509	6.98	1.71

[a]SA = Total surface area. [b]Overall variance (σ^2_{tot}). [c]Positive variance (σ^2_{+}). [d]Balance of charges (υ). [e]h_{50} [cm] = Height from where 50% probability of the dropped materials resulted in an explosion. [f]h_{50} [J] = Predicted impact sensitivities using 2.5 kg weight of a drop-hammer. * Experimentally measured impact sensitivity.

Table S4. The standard enthalpies of combustion $\Delta H_{f(combust)}$ for the title compounds was calculated by following equation

$$\Delta H_{f(combust)} = \Sigma\Delta H_{f\,(products)} - \Sigma\Delta H_{f\,(reactants)} \quad \text{(S14)}$$

RDX = $C_3H_6N_6O_6\,(s) + 1.5\,O_2\,(g) \longrightarrow 3CO_2\,(g) + 3H_2O\,(g) + 3N_2\,(g)$

HMX = $C_4H_8N_8O_8\,(s) + 2.0\,O_2\,(g) \longrightarrow 4CO_2\,(g) + 4H_2O\,(g) + 4N_2\,(g)$

CL-20 = $C_6H_6N_{12}O_{12}\,(s) + 1.5\,O_2\,(g) \longrightarrow 6CO_2\,(g) + 3H_2O\,(g) + 6N_2\,(g)$

AHC-12 = $C_8H_9N(s) + 10.25\,O_2\,(g) \longrightarrow 8CO_2\,(g) + 4.5H_2O\,(g) + 0.5N_2\,(g)$

AHC-13 = $C_8H_8N_2O_2(s) + 10.0\,O_2\,(g) \longrightarrow 8CO_2\,(g) + 4H_2O\,(g) + N_2\,(g)$

AHC-14 = $C_8H_9N_3O_2(s) + 10.25\,O_2\,(g) \longrightarrow 8CO_2\,(g) + 4.5H_2O\,(g) + 1.5N_2\,(g)$

AHC-15 = $C_9H_{10}N_2O_2(s) + 11.50\,O_2\,(g) \longrightarrow 9CO_2\,(g) + 5H_2O\,(g) + N_2\,(g)$

AHC-16 = $C_9H_{10}N_2O_3(s) + 11.50\,O_2\,(g) \longrightarrow 9CO_2\,(g) + 5H_2O\,(g) + N_2\,(g)$

AHC-17 = $C_9H_{10}N_4(s) + 11.50\,O_2\,(g) \longrightarrow 9CO_2\,(g) + 5H_2O\,(g) + 2N_2\,(g)$

AHC-18 = $C_9H_8N_4O_6(s) + 11.0\,O_2\,(g) \longrightarrow 9CO_2\,(g) + 4H_2O\,(g) + 2N_2\,(g)$

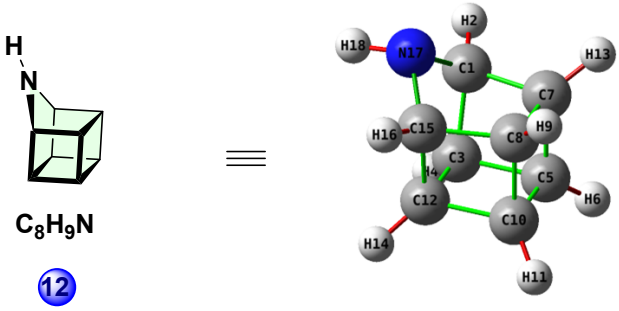
AHC-19 = $C_{10}H_{10}N_4O_6(s) + 12.50\,O_2\,(g) \longrightarrow 10CO_2\,(g) + 5H_2O\,(g) + 2N_2\,(g)$

AHC-20 = $C_8HN_9O_{16}(s) + 1.5\,O_2\,(g) \longrightarrow 8CO_2\,(g) + 0.5H_2O\,(g) + 4.5N_2\,(g)$

AHC-21 = $C_8N_{10}O_{18}(s) + 1.5\,O_2\,(g) \longrightarrow 8CO_2\,(g) + 5N_2\,(g)$

The standard enthalpy of formation for CO_2 ($\Delta H_{f\,(CO2)}$ = -393.51 kJmol^{-1}); H_2O ($\Delta H_{f\,(H2O)}$ = -243.015 kJmol^{-1}).

Table S5. Cartesian coordinates (in Å) for optimized structure **AHC-12** obtained using the B3LYP/6-311++G(d,p) level of theory



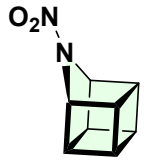
Optimized structure

```
Zero-point correction=                           0.152402 (Hartree/Particle)
Thermal correction to Energy=                    0.157396
Thermal correction to Enthalpy=                  0.158340
Thermal correction to Gibbs Free Energy=         0.123469
Sum of electronic and zero-point Energies=           -364.816590
Sum of electronic and thermal Energies=              -364.811596
Sum of electronic and thermal Enthalpies=            -364.810652
Sum of electronic and thermal Free Energies=         -364.845523
```

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.928741	-0.158059	1.631573
2	H	-0.270430	-0.213611	2.497536
3	C	-0.847653	1.121041	0.711061
4	H	-0.476555	2.072218	1.090614
5	C	-0.185995	0.284271	-0.438024
6	H	0.788588	0.482483	-0.879466
7	C	-0.568981	-1.003410	0.373092
8	C	-1.945536	-1.062643	-0.379082
9	H	-2.280607	-2.003831	-0.810563
10	C	-1.554503	0.224907	-1.186283
11	H	-1.720341	0.374305	-2.251269
12	C	-2.220934	1.062068	-0.040021
13	H	0.036152	-1.904146	0.455747
14	H	-2.802704	1.972001	-0.181401
15	C	-2.865359	-0.241319	0.572811
16	H	-3.943494	-0.371917	0.489491
17	N	-2.328167	-0.470327	1.912005
18	H	-2.733216	0.157235	2.603521

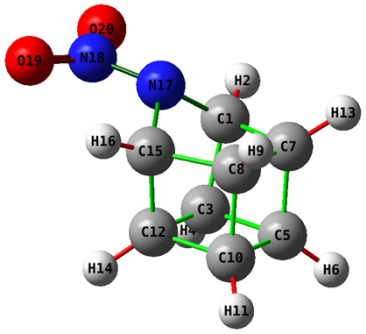
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S6. Cartesian coordinates (in Å) for optimized structure **AHC-13** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_8H_8N_2O_2$

13



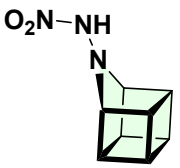
Optimized structure

```
Zero-point correction=                           0.154806 (Hartree/Particle)
Thermal correction to Energy=                    0.162278
Thermal correction to Enthalpy=                  0.163222
Thermal correction to Gibbs Free Energy=         0.121814
Sum of electronic and zero-point Energies=           -569.363292
Sum of electronic and thermal Energies=              -569.355820
Sum of electronic and thermal Enthalpies=            -569.354876
Sum of electronic and thermal Free Energies=         -569.396284
```

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.893784	-0.093093	1.622254
2	H	-0.258161	-0.136656	2.499147
3	C	-0.813622	1.147420	0.664274
4	H	-0.426741	2.101104	1.015689
5	C	-0.173469	0.260563	-0.460013
6	H	0.804931	0.423143	-0.905371
7	C	-0.580844	-0.990932	0.395166
8	C	-1.963045	-1.045344	-0.353972
9	H	-2.317110	-1.993822	-0.751183
10	C	-1.545185	0.206164	-1.203640
11	H	-1.714296	0.323310	-2.271217
12	C	-2.192655	1.093282	-0.083447
13	H	0.001882	-1.902414	0.506368
14	H	-2.755864	2.009240	-0.245957
15	C	-2.874298	-0.171312	0.548251
16	H	-3.951222	-0.282714	0.496434
17	N	-2.316169	-0.353888	1.898035
18	N	-2.910552	0.372019	2.940827
19	O	-4.109946	0.592909	2.849087
20	O	-2.196000	0.665750	3.888881

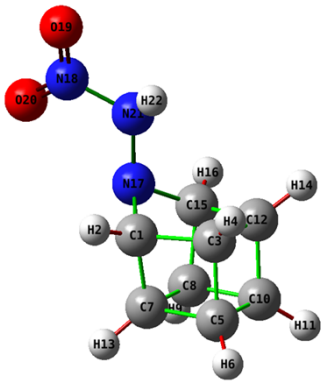
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S7. Cartesian coordinates (in Å) for optimized structure **AHC-14** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_8H_9N_3O_2$

14



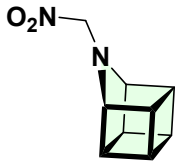
Optimized structure

```
Zero-point correction=                           0.170998 (Hartree/Particle)
Thermal correction to Energy=                    0.179752
Thermal correction to Enthalpy=                  0.180696
Thermal correction to Gibbs Free Energy=         0.135726
Sum of electronic and zero-point Energies=          -624.682197
Sum of electronic and thermal Energies=             -624.673444
Sum of electronic and thermal Enthalpies=           -624.672499
Sum of electronic and thermal Free Energies=        -624.717469
```

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-1.375959	-0.410180	1.888755
2	H	-1.178262	-0.723766	2.912128
3	C	-0.695128	0.899693	1.332291
4	H	-0.338168	1.686745	1.994512
5	C	0.212976	0.042564	0.383219
6	H	1.300313	0.034437	0.399873
7	C	-0.705806	-1.181954	0.723281
8	C	-1.632653	-0.817748	-0.497142
9	H	-1.926029	-1.600914	-1.192149
10	C	-0.703977	0.403324	-0.827127
11	H	-0.382650	0.696531	-1.823750
12	C	-1.617552	1.261367	0.115618
13	H	-0.374555	-2.209630	0.851925
14	H	-1.902643	2.297366	-0.056816
15	C	-2.689047	0.108424	0.156640
16	H	-3.648925	0.256810	-0.330808
17	N	-2.804625	-0.379321	1.538367
18	N	-4.454343	-0.312011	3.254977
19	O	-4.803656	0.346713	4.225326
20	O	-4.791913	-1.435028	2.965970
21	N	-3.615986	0.404511	2.343112
22	H	-3.182827	1.149589	2.887789

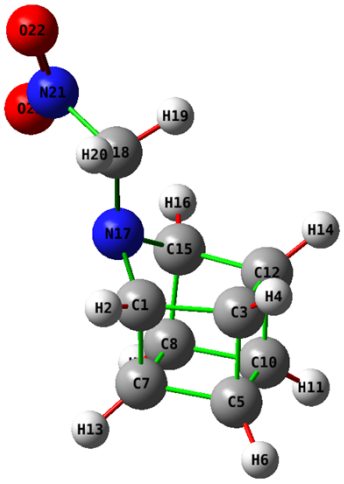
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S8. Cartesian coordinates (in Å) for optimized structure **AHC-15** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_9H_{10}N_2O_2$

15



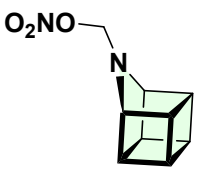
Optimized structure

```
Zero-point correction=                           0.182761 (Hartree/Particle)
Thermal correction to Energy=                    0.191859
Thermal correction to Enthalpy=                  0.192803
Thermal correction to Gibbs Free Energy=         0.146068
Sum of electronic and zero-point Energies=           -608.666134
Sum of electronic and thermal Energies=              -608.657036
Sum of electronic and thermal Enthalpies=            -608.656092
Sum of electronic and thermal Free Energies=         -608.702827
```

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.790181	-0.040923	1.578049
2	H	-0.065840	-0.047214	2.391239
3	C	-0.804165	1.184273	0.583094
4	H	-0.412538	2.158482	0.871664
5	C	-0.235329	0.284117	-0.567444
6	H	0.696244	0.461610	-1.099910
7	C	-0.534620	-0.955129	0.347834
8	C	-1.969324	-1.067407	-0.280871
9	H	-2.327516	-2.034995	-0.624809
10	C	-1.661768	0.173246	-1.190610
11	H	-1.921560	0.261145	-2.242993
12	C	-2.236475	1.072953	-0.041530
13	H	0.082725	-1.846757	0.433616
14	H	-2.833905	1.971109	-0.188734
15	C	-2.818082	-0.200503	0.688990
16	H	-3.894565	-0.351619	0.712015
17	N	-2.165363	-0.328416	1.993247
18	C	-2.682195	0.427186	3.076986
19	H	-3.219200	1.348531	2.813022
20	H	-1.914973	0.663141	3.811403
21	N	-3.747950	-0.356990	3.883555
22	O	-3.978915	0.081317	5.001226
23	O	-4.306404	-1.297695	3.356004

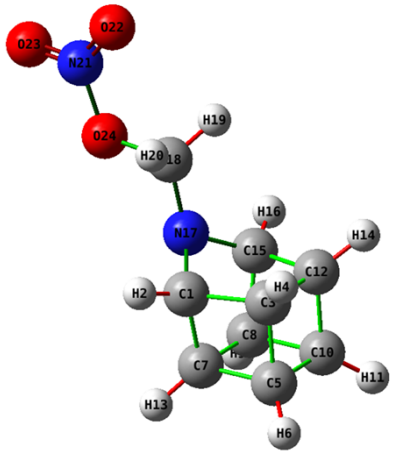
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S9. Cartesian coordinates (in Å) for optimized structure **AHC-16** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_9H_{10}N_2O_3$

16



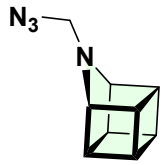
Optimized structure

Zero-point correction=	0.186649 (Hartree/Particle)
Thermal correction to Energy=	0.196824
Thermal correction to Enthalpy=	0.197768
Thermal correction to Gibbs Free Energy=	0.147486
Sum of electronic and zero-point Energies=	-683.866092
Sum of electronic and thermal Energies=	-683.855917
Sum of electronic and thermal Enthalpies=	-683.854972
Sum of electronic and thermal Free Energies=	-683.905255

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.901757	0.261091	1.590980
2	H	-0.262999	0.452758	2.451119
3	C	-0.927456	1.308833	0.410757
4	H	-0.654224	2.350621	0.570738
5	C	-0.172773	0.305972	-0.528917
6	H	0.787262	0.493790	-1.004049
7	C	-0.450580	-0.801249	0.547554
8	C	-1.804160	-1.151735	-0.170292
9	H	-2.041617	-2.192425	-0.380310
10	C	-1.516873	-0.042388	-1.241535
11	H	-1.679482	-0.145369	-2.311893
12	C	-2.276927	0.959624	-0.304968
13	H	0.228840	-1.604567	0.824471
14	H	-2.934497	1.760405	-0.639224
15	C	-2.814808	-0.234463	0.576165
16	H	-3.873542	-0.483212	0.536301
17	N	-2.279295	-0.085728	1.925669
18	C	-2.989474	0.620612	2.913796
19	H	-3.899943	1.100481	2.550404
20	H	-2.373614	1.346296	3.445334
21	N	-4.166256	0.107639	4.986509
22	O	-4.365396	1.306174	5.013586
23	O	-4.525599	-0.732001	5.768511
24	O	-3.420050	-0.404433	3.917847

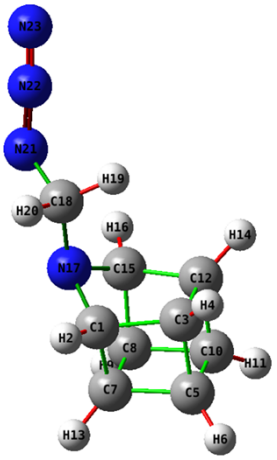
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S10. Cartesian coordinates (in Å) for optimized structure **AHC-17** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_9H_{10}N_4$

17



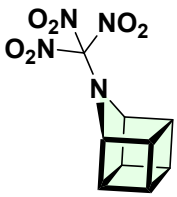
Optimized structure

Zero-point correction=	0.183390 (Hartree/Particle)
Thermal correction to Energy=	0.192526
Thermal correction to Enthalpy=	0.193470
Thermal correction to Gibbs Free Energy=	0.147222
Sum of electronic and zero-point Energies=	-567.727732
Sum of electronic and thermal Energies=	-567.718596
Sum of electronic and thermal Enthalpies=	-567.717652
Sum of electronic and thermal Free Energies=	-567.763899

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.716774	-0.080938	1.566781
2	H	0.059921	-0.064979	2.330714
3	C	-0.890598	1.191452	0.642534
4	H	-0.556777	2.179308	0.955925
5	C	-0.327193	0.398260	-0.586369
6	H	0.550532	0.678936	-1.164598
7	C	-0.466598	-0.906327	0.274358
8	C	-1.925072	-1.105562	-0.270641
9	H	-2.228061	-2.080061	-0.647495
10	C	-1.777953	0.200494	-1.127377
11	H	-2.110693	0.318370	-2.156327
12	C	-2.346307	0.992930	0.100357
13	H	0.226225	-1.745234	0.272341
14	H	-3.022162	1.843851	0.035448
15	C	-2.772655	-0.361233	0.797307
16	H	-3.831670	-0.594550	0.880018
17	N	-2.029622	-0.505858	2.050076
18	C	-2.530412	0.263498	3.163107
19	H	-2.730468	1.321149	2.911242
20	H	-1.785228	0.234944	3.965579
21	N	-3.788131	-0.366693	3.633499
22	N	-4.483737	0.329994	4.367631
23	N	-5.206894	0.878308	5.050655

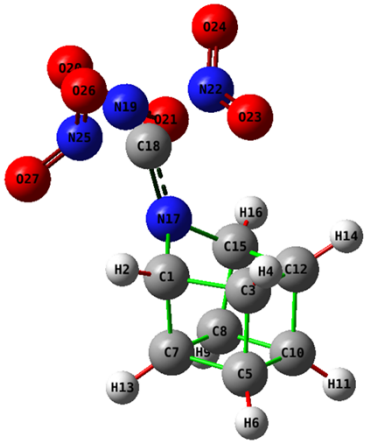
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S11. Cartesian coordinates (in Å) for optimized structure **AHC-18** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_9H_8N_4O_6$

18



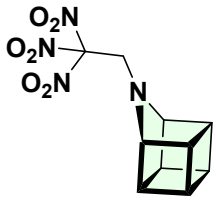
Optimized structure

```
Zero-point correction=                           0.185672 (Hartree/Particle)
Thermal correction to Energy=                    0.200167
Thermal correction to Enthalpy=                  0.201111
Thermal correction to Gibbs Free Energy=         0.142237
Sum of electronic and zero-point Energies=          -1017.745535
Sum of electronic and thermal Energies=             -1017.731040
Sum of electronic and thermal Enthalpies=           -1017.730096
Sum of electronic and thermal Free Energies=        -1017.788970
```

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.858160	0.497055	1.401563
2	H	-0.222233	0.923398	2.170292
3	C	-1.105714	1.299886	0.084749
4	H	-1.009155	2.381717	0.066271
5	C	-0.231235	0.280537	-0.727304
6	H	0.671251	0.527791	-1.280053
7	C	-0.292992	-0.659043	0.528994
8	C	-1.593268	-1.326612	-0.040050
9	H	-1.671811	-2.411017	-0.060337
10	C	-1.525210	-0.382900	-1.292154
11	H	-1.708039	-0.690268	-2.318461
12	C	-2.402924	0.635291	-0.481381
13	H	0.512987	-1.288276	0.899009
14	H	-3.188731	1.264730	-0.890507
15	C	-2.724590	-0.463768	0.586368
16	H	-3.724583	-0.874822	0.645414
17	N	-2.166978	-0.010049	1.884470
18	C	-2.880011	0.498291	2.920267
19	N	-3.882388	-0.536190	3.576173
20	O	-3.916605	-0.563550	4.784358
21	O	-4.522413	-1.217972	2.803924
22	N	-3.834057	1.775296	2.598071
23	O	-3.367449	2.548143	1.788465
24	O	-4.914398	1.827223	3.138887
25	N	-1.951199	0.979436	4.079028
26	O	-2.165077	2.082475	4.530589
27	O	-1.096317	0.191830	4.418534

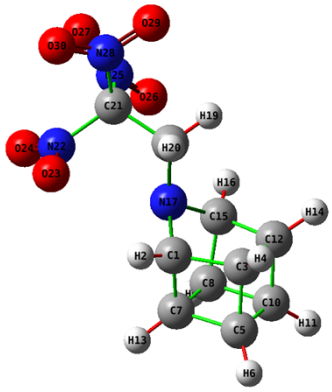
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S12. Cartesian coordinates (in Å) for optimized structure **AHC-19** obtained using the B3LYP/6-311++G(d,p) level of theory



$C_{10}H_{10}N_4O_6$

19



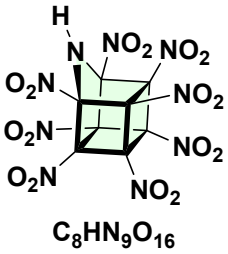
Optimized structure

```
Zero-point correction=                           0.214582 (Hartree/Particle)
Thermal correction to Energy=                    0.230114
Thermal correction to Enthalpy=                  0.231058
Thermal correction to Gibbs Free Energy=         0.169359
Sum of electronic and zero-point Energies=          -1057.036601
Sum of electronic and thermal Energies=             -1057.021069
Sum of electronic and thermal Enthalpies=           -1057.020125
Sum of electronic and thermal Free Energies=        -1057.081823
```

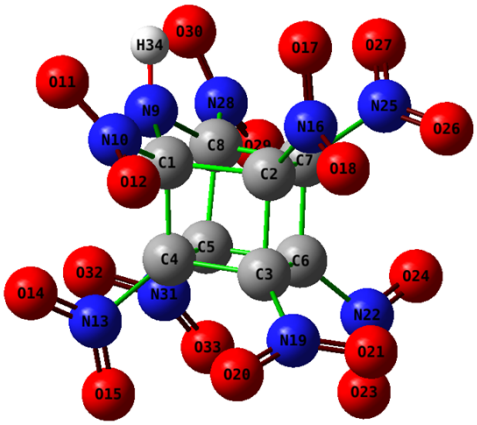
Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.924356	0.104753	1.682634
2	H	-0.344487	0.250442	2.591508
3	C	-0.944996	1.251204	0.600355
4	H	-0.735612	2.287421	0.860903
5	C	-0.083974	0.371742	-0.372120
6	H	0.889357	0.648578	-0.770302
7	C	-0.359719	-0.838689	0.587680
8	C	-1.648079	-1.193232	-0.237082
9	H	-1.817492	-2.221439	-0.548717
10	C	-1.364360	0.019413	-1.191856
11	H	-1.460308	0.002898	-2.274922
12	C	-2.230024	0.896980	-0.222167
13	H	0.348829	-1.624823	0.838662
14	H	-2.910905	1.688238	-0.531694
15	C	-2.747080	-0.396859	0.515571
16	H	-3.783670	-0.695237	0.388022
17	N	-2.303101	-0.349494	1.915349
18	C	-3.094772	0.453047	2.829880
19	H	-3.961979	0.918524	2.357287
20	H	-2.503675	1.254688	3.281241
21	C	-3.624352	-0.397257	3.996988
22	N	-2.520091	-1.338738	4.512188
23	O	-1.488551	-0.772742	4.808755
24	O	-2.757613	-2.522930	4.557658
25	N	-4.859878	-1.262975	3.642878
26	O	-5.032848	-1.500635	2.467038
27	O	-5.540616	-1.625337	4.577332
28	N	-4.095951	0.492656	5.162626
29	O	-4.842447	1.390222	4.814347
30	O	-3.707655	0.246029	6.279368

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S13. Cartesian coordinates (in Å) for optimized structure **AHC-20** obtained using the B3LYP/6-311++G(d,p) level of theory



20



Optimized structure

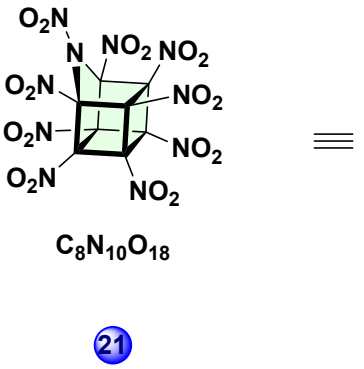
```
Zero-point correction=                           0.166728 (Hartree/Particle)
Thermal correction to Energy=                    0.194315
Thermal correction to Enthalpy=                  0.195259
Thermal correction to Gibbs Free Energy=         0.107722
Sum of electronic and zero-point Energies=          -2001.177272
Sum of electronic and thermal Energies=             -2001.149685
Sum of electronic and thermal Enthalpies=           -2001.148741
Sum of electronic and thermal Free Energies=        -2001.236278
```

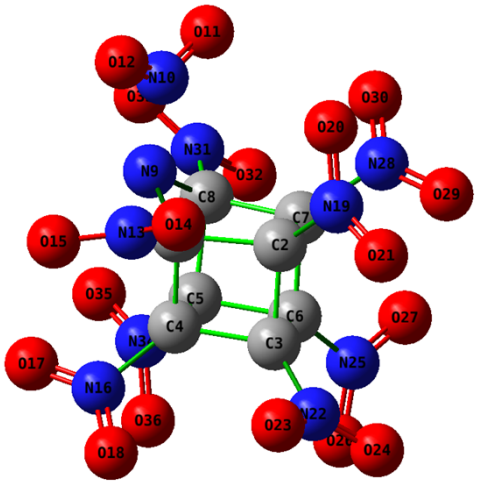
Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.981703	-0.186737	1.654706
2	C	-0.821840	1.093684	0.701071
3	C	-0.164072	0.242893	-0.432008
4	C	-0.586065	-1.022426	0.388272
5	C	-1.949745	-1.035527	-0.389817
6	C	-1.522583	0.238702	-1.187148
7	C	-2.193395	1.074308	-0.049642
8	C	-2.865964	-0.223178	0.599132
9	N	-2.351556	-0.457673	1.903778
10	N	-0.076668	-0.200298	2.862324
11	O	-0.579450	-0.485894	3.923685
12	O	1.075270	0.117935	2.632341
13	N	0.196937	-2.302218	0.466345
14	O	0.499630	-2.696274	1.570615
15	O	0.435052	-2.812676	-0.609846
16	N	-0.331263	2.376464	1.286867
17	O	-1.070111	2.821960	2.152815
18	O	0.716970	2.824654	0.891420
19	N	1.179898	0.520710	-1.018505
20	O	2.097149	-0.160949	-0.609712
21	O	1.209519	1.422686	-1.827858
22	N	-1.737236	0.419914	-2.653331
23	O	-0.890124	-0.069125	-3.367856
24	O	-2.748142	1.013152	-2.971710
25	N	-2.913262	2.374427	-0.258904
26	O	-2.259974	3.236674	-0.810417
27	O	-4.054383	2.439293	0.145931
28	N	-4.360385	-0.384243	0.468081
29	O	-4.763896	-0.554552	-0.666428

30	O	-5.001223	-0.315355	1.491646
31	N	-2.449033	-2.326410	-0.976114
32	O	-2.704876	-3.180399	-0.148082
33	O	-2.556693	-2.383570	-2.178039
34	H	-2.800353	0.033255	2.674087

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S14. Cartesian coordinates (in Å) for optimized structure **AHC-21** obtained using the B3LYP/6-311++G(d,p) level of theory





Optimized structure

```
Zero-point correction=                           0.167327 (Hartree/Particle)
Thermal correction to Energy=                    0.197563
Thermal correction to Enthalpy=                  0.198508
Thermal correction to Gibbs Free Energy=         0.104960
Sum of electronic and zero-point Energies=          -2205.669024
Sum of electronic and thermal Energies=             -2205.638788
Sum of electronic and thermal Enthalpies=           -2205.637843
Sum of electronic and thermal Free Energies=        -2205.731391
```

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.911599	-0.158132	1.636565
2	C	-0.848453	1.121039	0.708751
3	C	-0.206222	0.308403	-0.463627
4	C	-0.570365	-0.983715	0.349856
5	C	-1.967289	-1.029028	-0.344647
6	C	-1.595835	0.258899	-1.167575
7	C	-2.252640	1.070003	-0.005396
8	C	-2.880183	-0.226776	0.645262
9	N	-2.298019	-0.457396	1.958379
10	N	-2.836848	0.428943	3.074613
11	O	-3.805528	1.078236	2.801272
12	O	-2.227129	0.323501	4.100077
13	N	0.097775	-0.294480	2.782999
14	O	0.759880	0.690510	3.027230
15	O	0.154630	-1.389571	3.288417
16	N	0.188479	-2.290248	0.452589
17	O	-0.459392	-3.199836	0.928509
18	O	1.333185	-2.297836	0.065823

19	N	-0.403064	2.454703	1.244494
20	O	-1.124796	2.882519	2.126523
21	O	0.578056	2.959272	0.758339
22	N	1.132648	0.674125	-1.018317
23	O	2.060834	0.496375	-0.258704
24	O	1.144268	1.149979	-2.132891
25	N	-1.884587	0.421549	-2.629025
26	O	-1.197595	-0.251706	-3.366239
27	O	-2.782317	1.184821	-2.919937
28	N	-2.961658	2.385233	-0.228387
29	O	-2.259703	3.225300	-0.760947
30	O	-4.109397	2.480682	0.127703
31	N	-4.364778	-0.499275	0.456643
32	O	-4.750149	-0.241120	-0.668310
33	O	-4.980298	-0.969549	1.375774
34	N	-2.385211	-2.347212	-0.955487
35	O	-3.394388	-2.860556	-0.532440
36	O	-1.629625	-2.755776	-1.813769

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

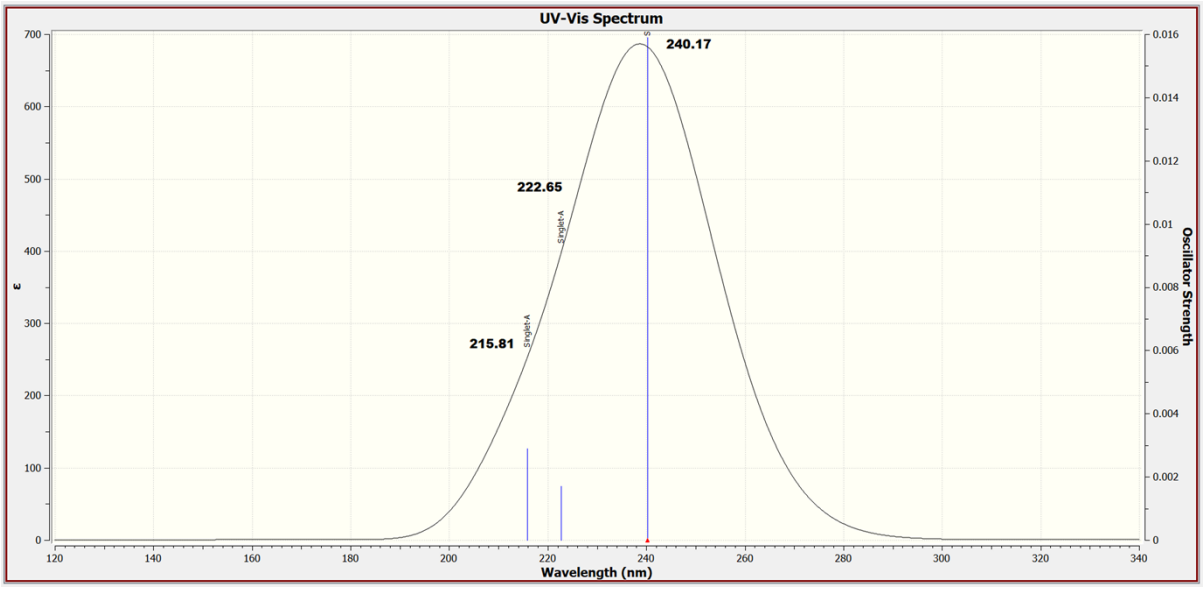


Figure S4. Computed UV- spectrum for compound **AHC-12**.

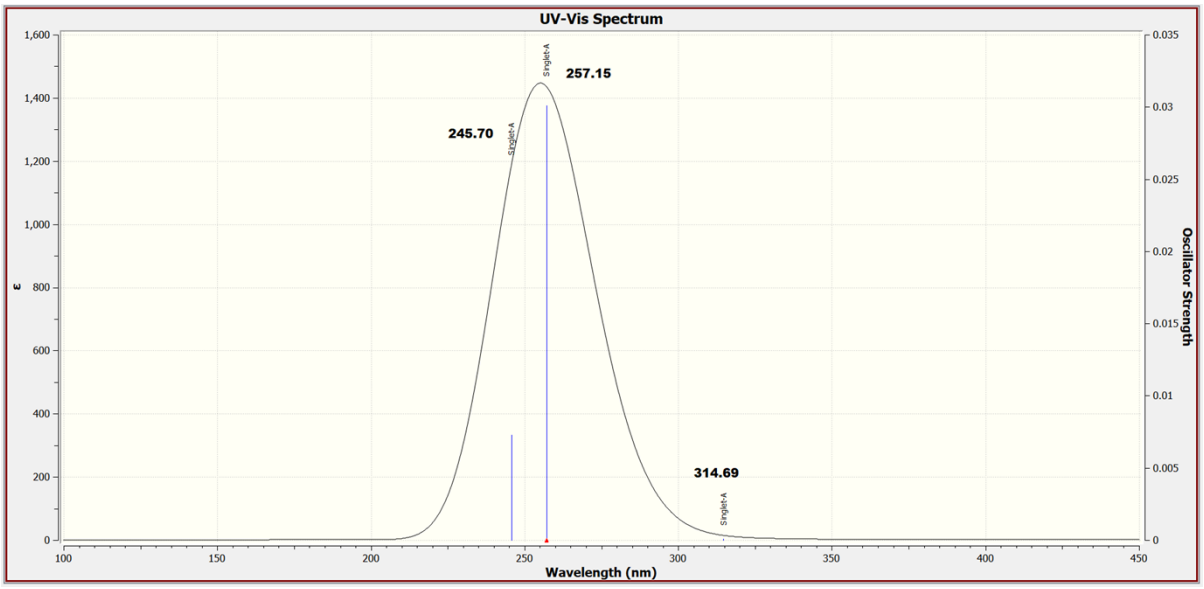


Figure S5. Computed UV- spectrum for compound **AHC-13**.

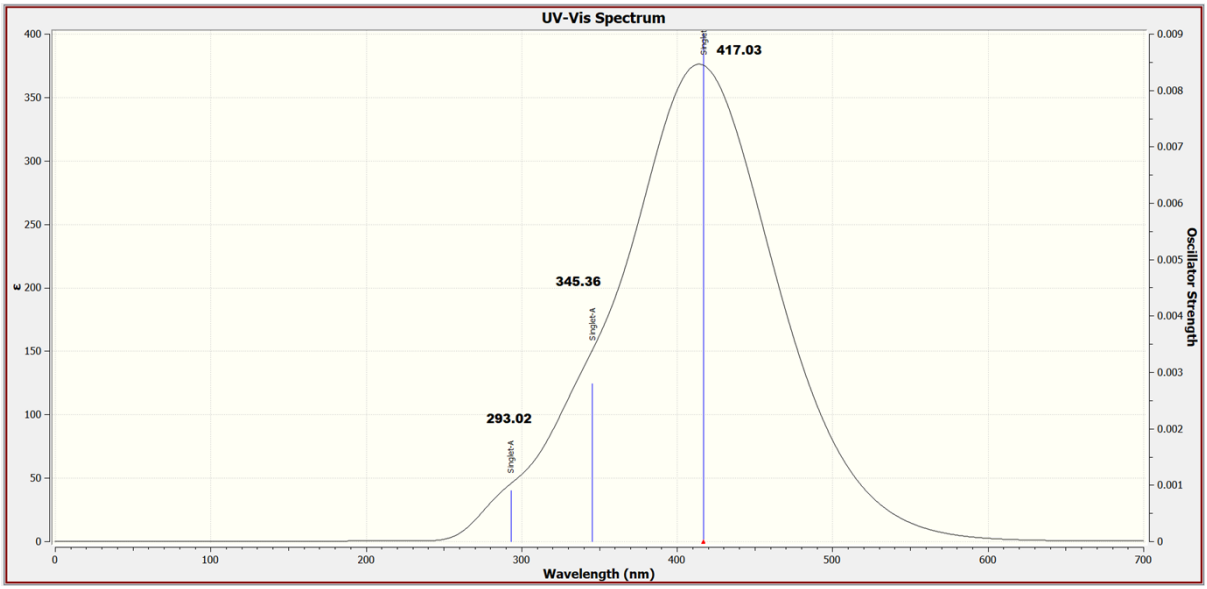


Figure S6. Computed UV- spectrum for compound **AHC-14**.

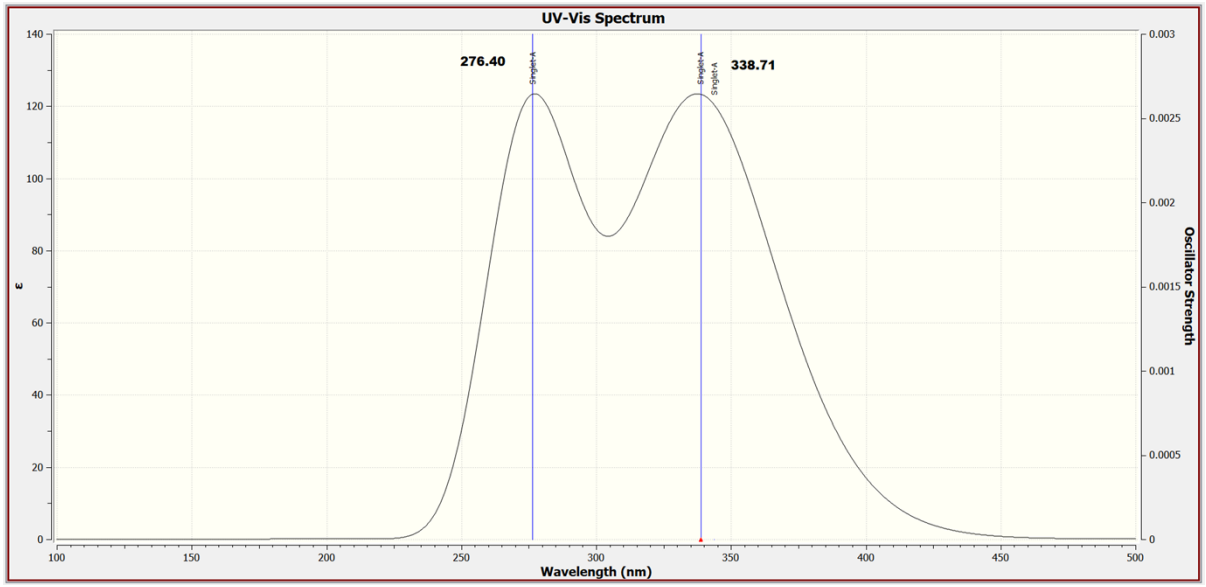


Figure S7. Computed UV- spectrum for compound **AHC-15**.

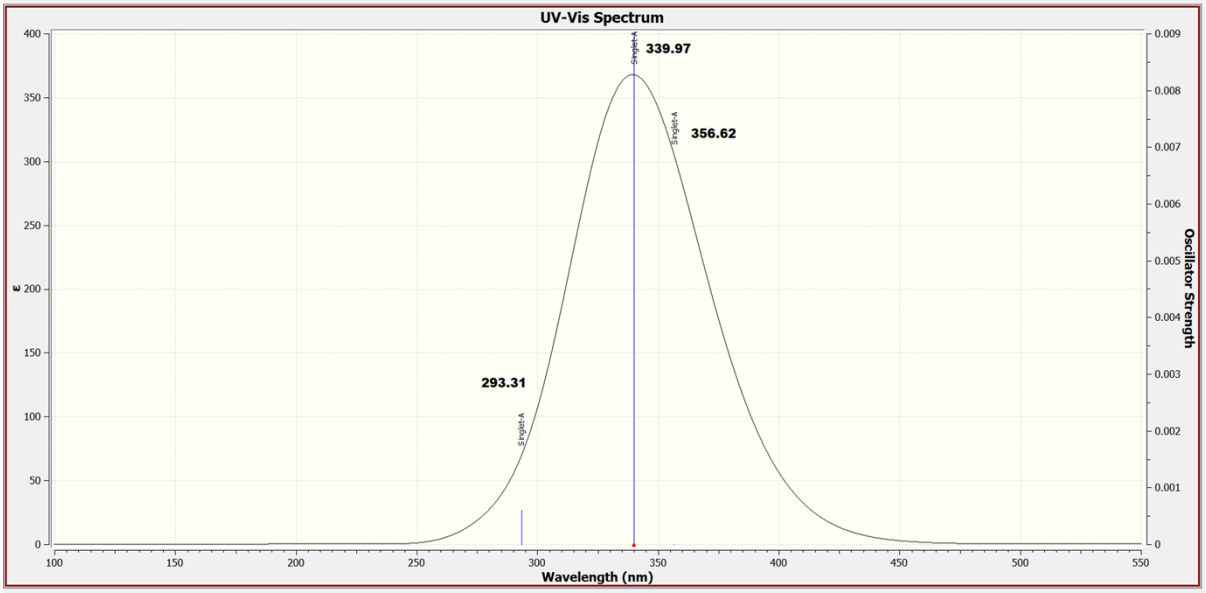


Figure S8. Computed UV- spectrum for compound **AHC-16**.

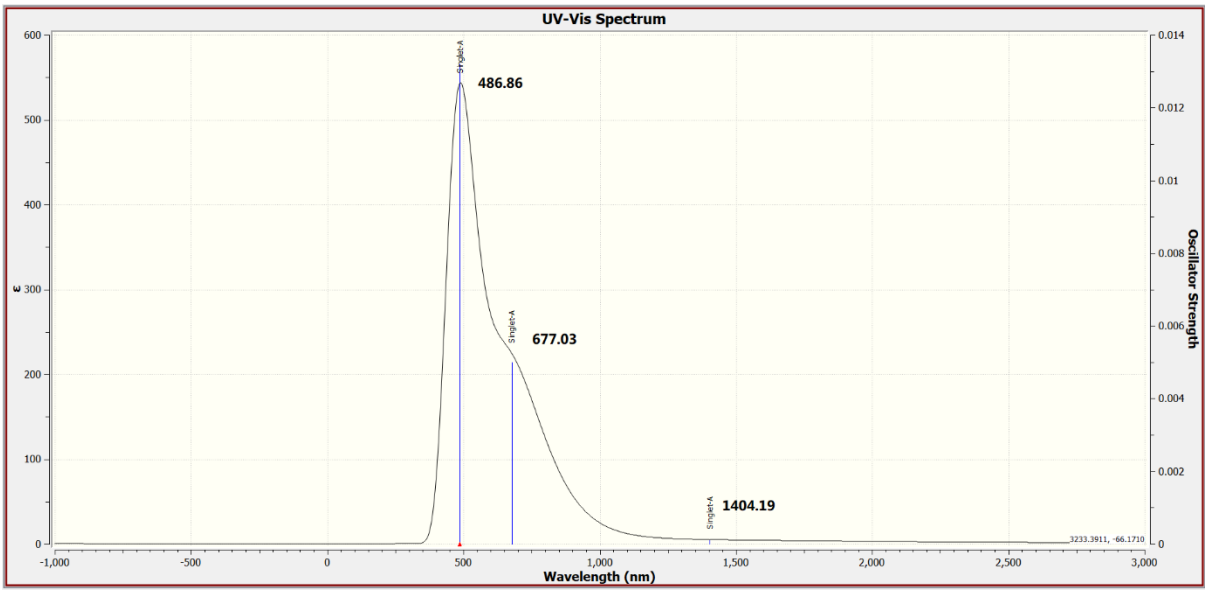


Figure S9. Computed UV- spectrum for compound **AHC-17**.

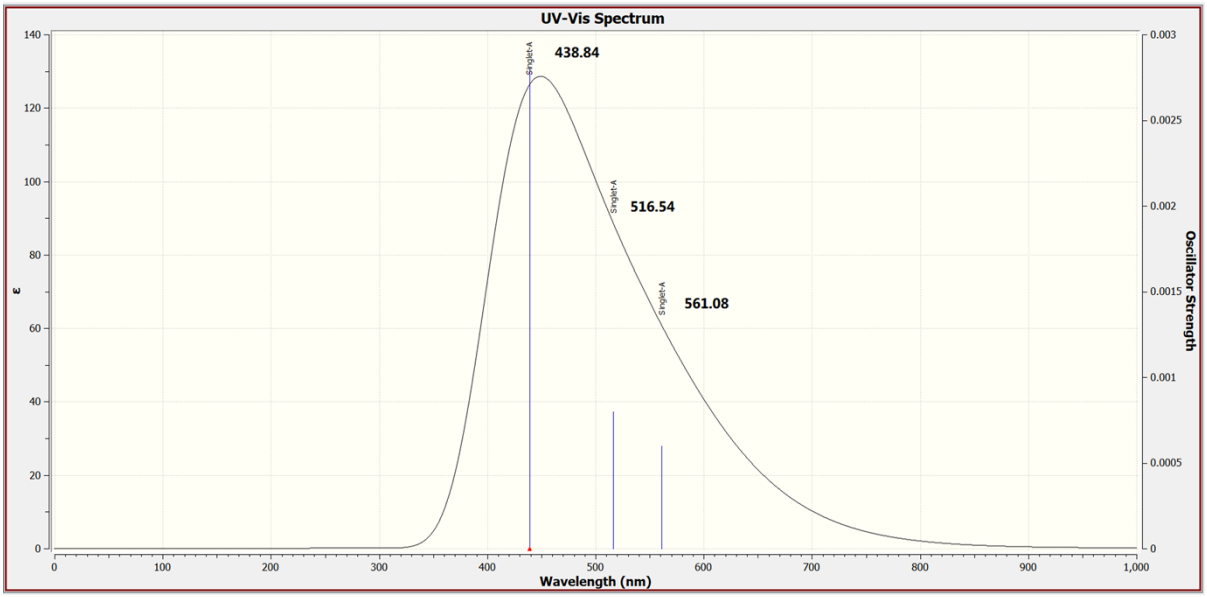


Figure S10. Computed UV- spectrum for compound **AHC-18.**

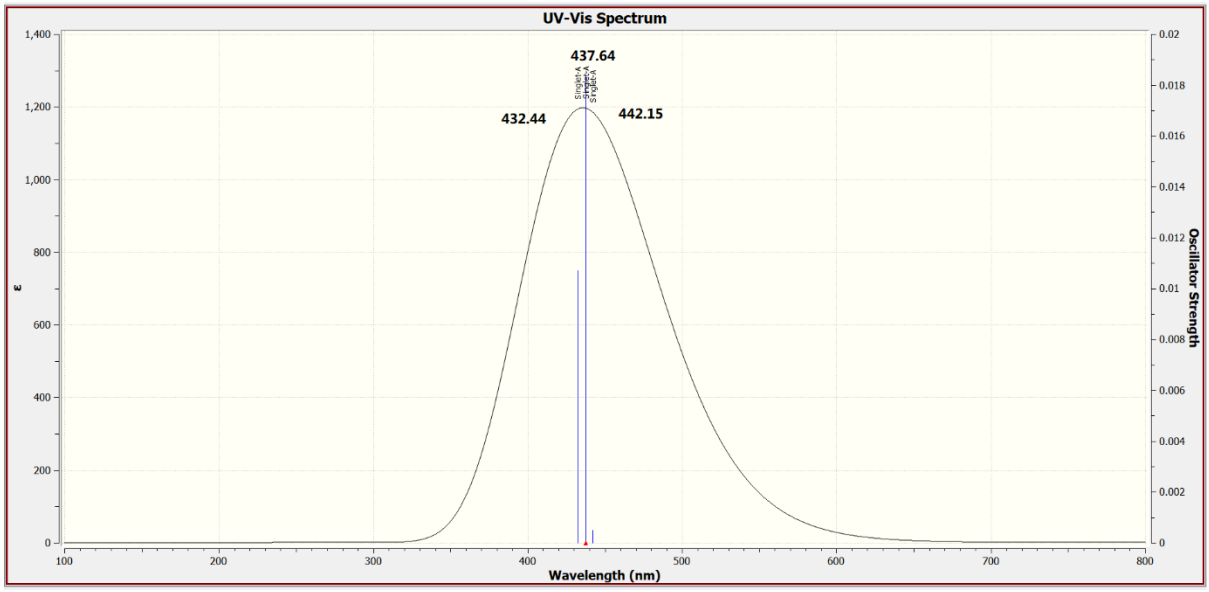


Figure S11. Computed UV- spectrum for compound **AHC-19.**

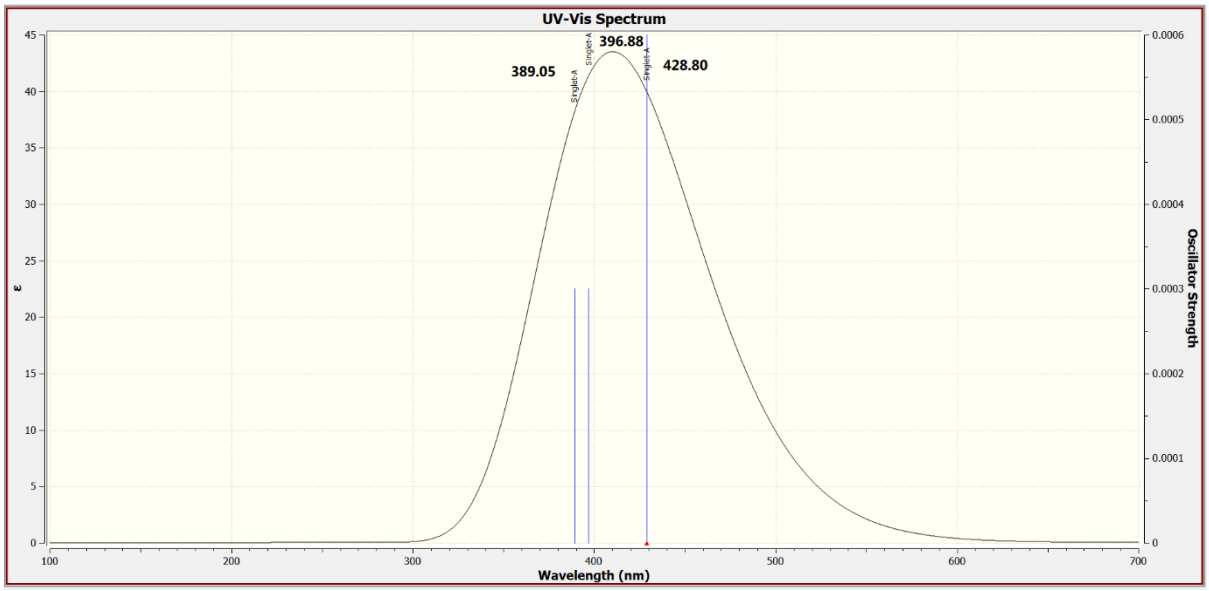


Figure S12. Computed UV- spectrum for compound **AHC-20.**

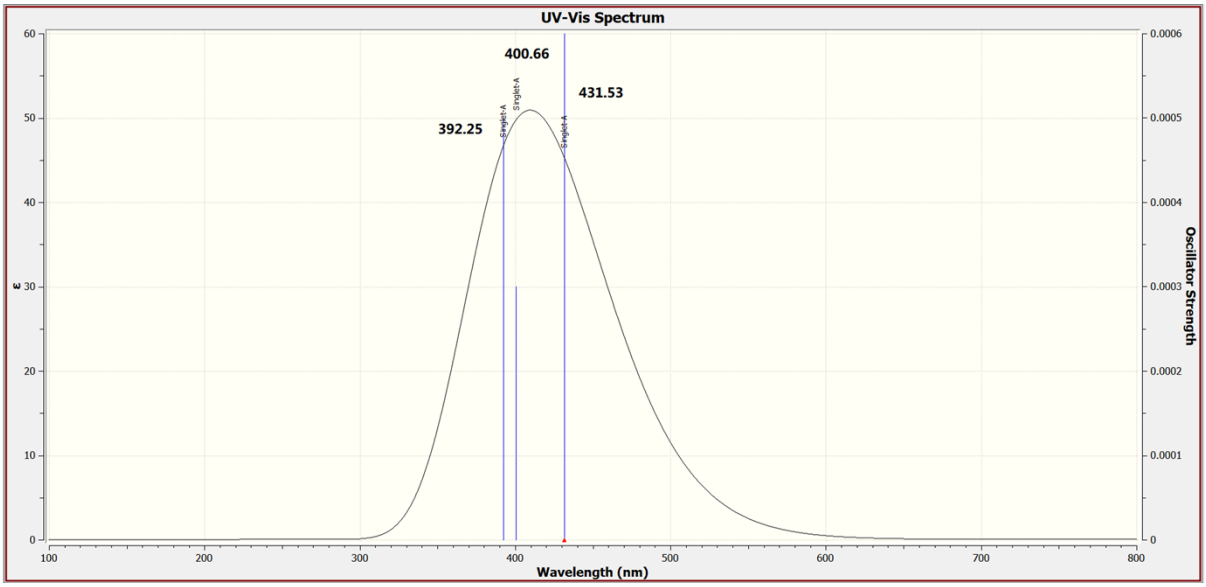


Figure S13. Computed UV- spectrum for compound **AHC-21.**

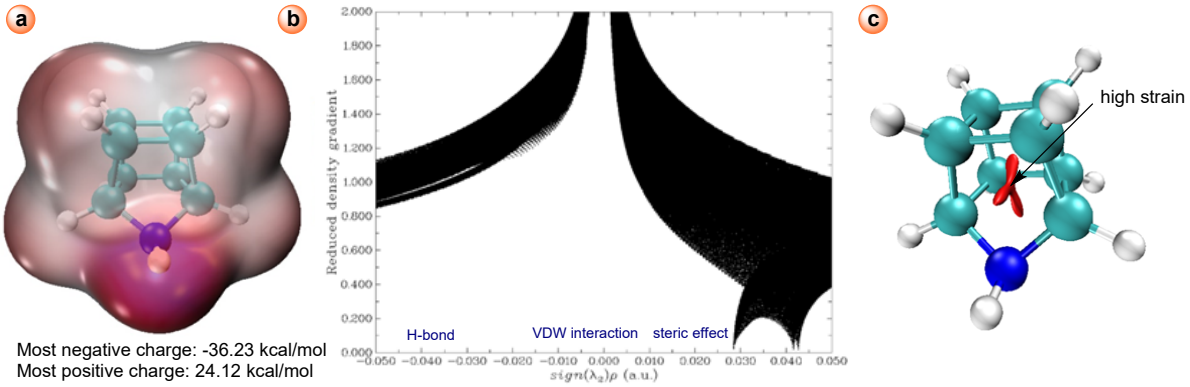


Figure S14. Computed electrostatic potential (ESP) maps of **AHC-12**. Scatter diagram of **AHC-12**. Rreduced density gradient (RDG) of **AHC-12,** calculated at B3LYP/6-311++G(d,p) level.

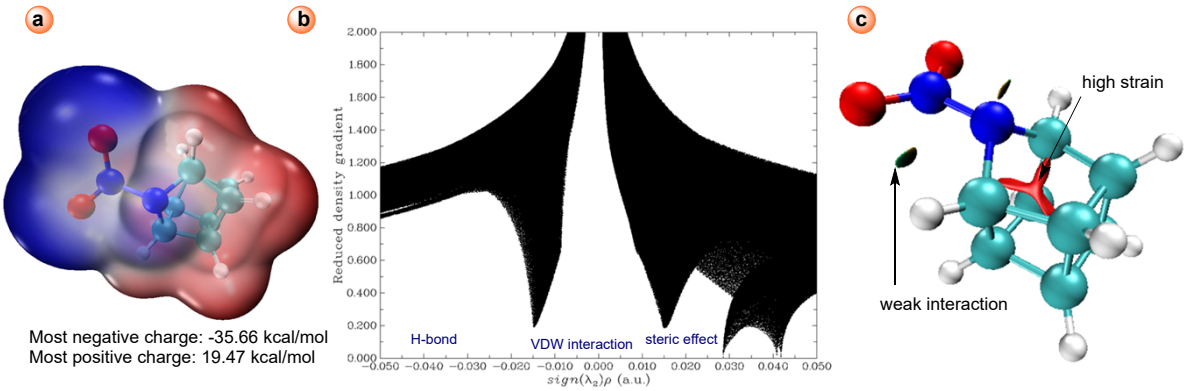


Figure S15. Computed electrostatic potential (ESP) maps of **AHC-13**. Scatter diagram of **AHC-13**. Rreduced density gradient (RDG) of **AHC-13,** calculated at B3LYP/6-311++G(d,p) level.

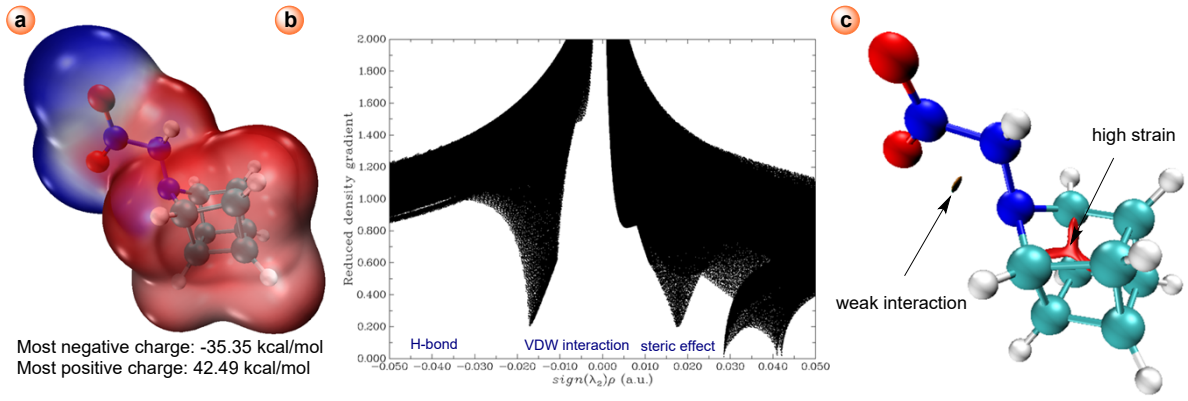


Figure S16. Computed electrostatic potential (ESP) maps of **AHC-14**. Scatter diagram of **AHC-14**. Rreduced density gradient (RDG) of **AHC-14,** calculated at B3LYP/6-311++G(d,p) level.

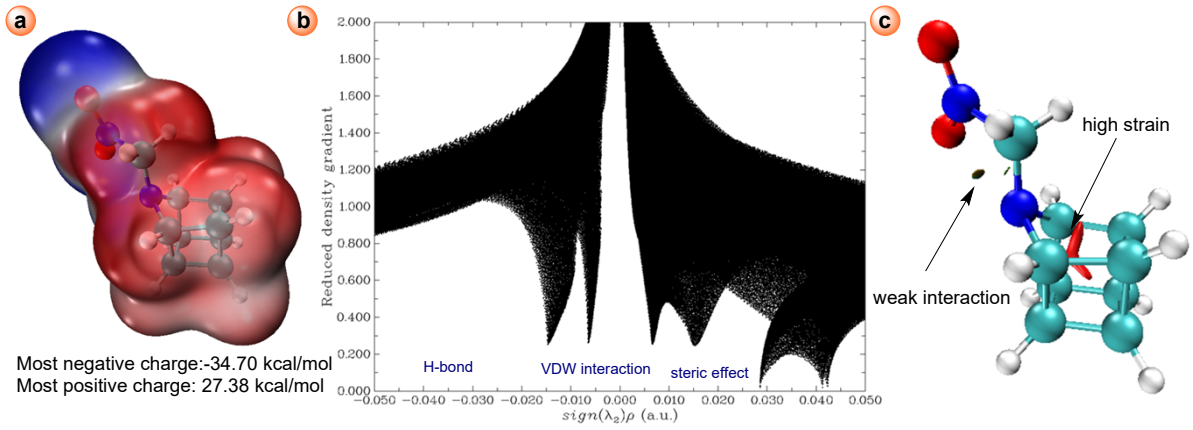


Figure S17. Computed electrostatic potential (ESP) maps of **AHC-15**. Scatter diagram of **AHC-15**. Rreduced density gradient (RDG) of **AHC-15,** calculated at B3LYP/6-311++G(d,p) level.

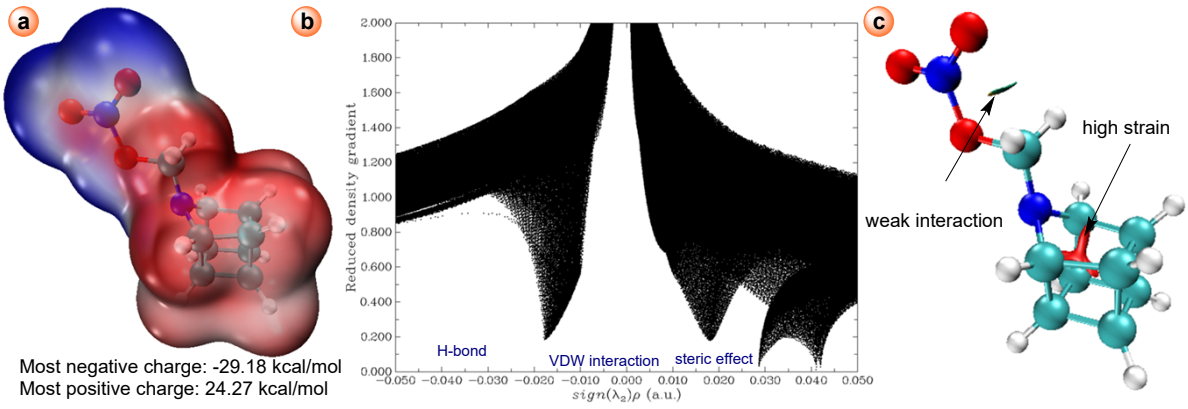


Figure S18. Computed electrostatic potential (ESP) maps of **AHC-16**. Scatter diagram of **AHC-16**. Rreduced density gradient (RDG) of **AHC-16,** calculated at B3LYP/6-311++G(d,p) level.

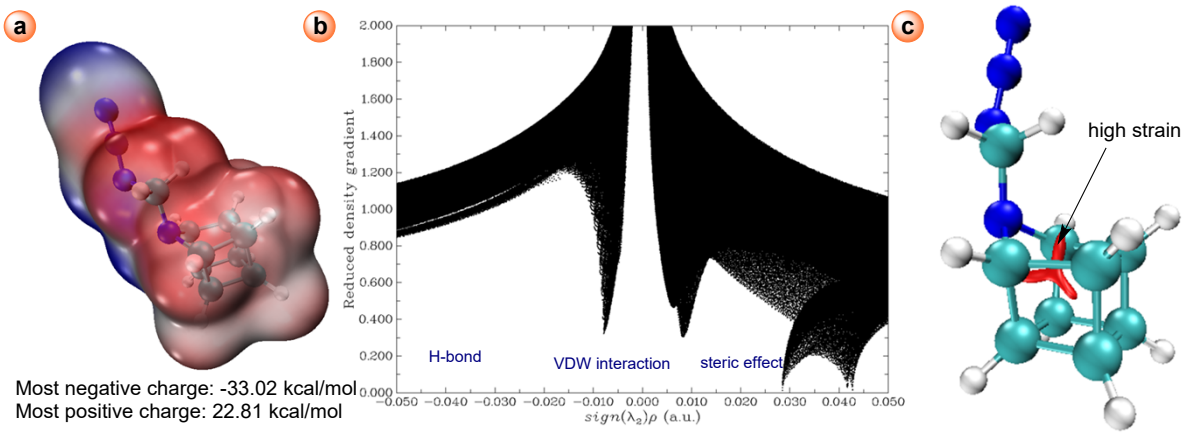


Figure S19. Computed electrostatic potential (ESP) maps of **AHC-17**. Scatter diagram of **AHC-17**. Rreduced density gradient (RDG) of **AHC-17,** calculated at B3LYP/6-311++G(d,p) level.

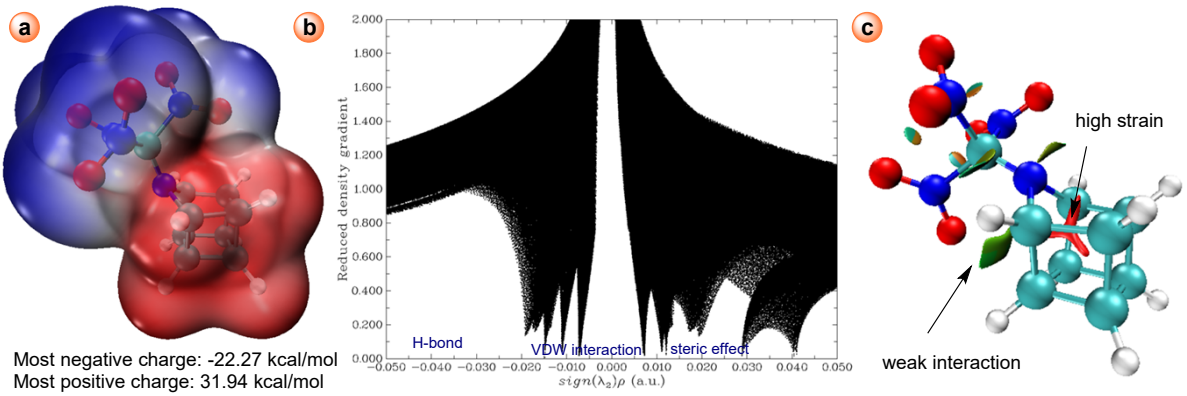


Figure S20. Computed electrostatic potential (ESP) maps of **AHC-18**. Scatter diagram of **AHC-18**. Rreduced density gradient (RDG) of **AHC-18,** calculated at B3LYP/6-311++G(d,p) level.

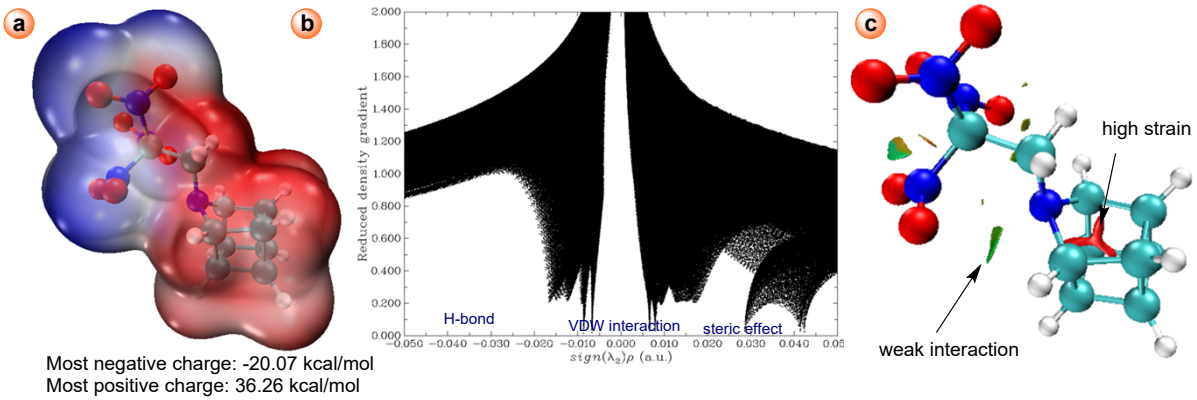


Figure S21. Computed electrostatic potential (ESP) maps of **AHC-19**. Scatter diagram of **AHC-19**. Rreduced density gradient (RDG) of **AHC-19,** calculated at B3LYP/6-311++G(d,p) level.

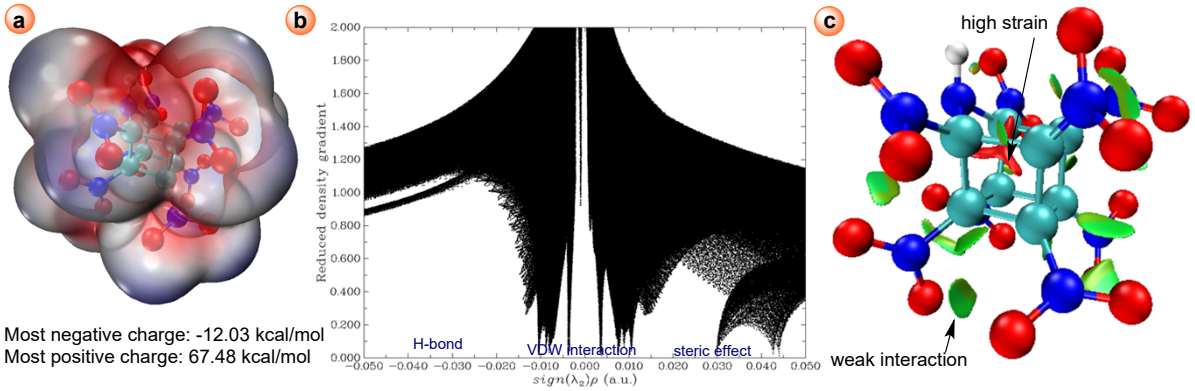


Figure S22. Computed electrostatic potential (ESP) maps of **AHC-20**. Scatter diagram of **AHC-20**. Rreduced density gradient (RDG) of **AHC-20,** calculated at B3LYP/6-311++G(d,p) level.

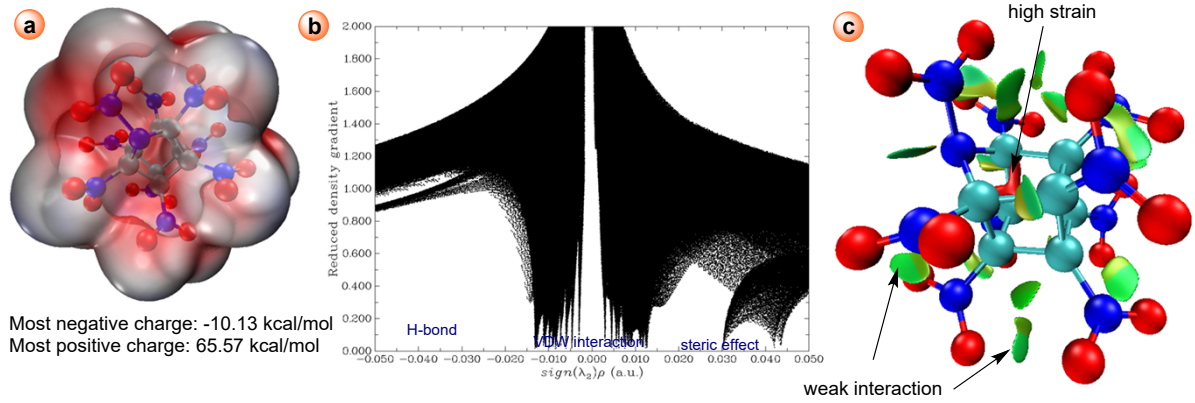


Figure S23. Computed electrostatic potential (ESP) maps of **AHC-21**. Scatter diagram of **AHC-21**. Rreduced density gradient (RDG) of **AHC-21,** calculated at B3LYP/6-311++G(d,p) level.

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