

Supporting Information

Tetracyclo(9-methyl-2,7-carbazole) as a Promising Nanohoop for Gas Trapping: A Multiscale Study

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Table S1. Physical parameters such as bond length, bond angle of the isolated guest molecule and the TCC entrapped guest molecules along with the NBO charge transfer values. The negative and positive values reveal the charge transfer from host to guest and guest to host respectively.

Gas Molecules	BLGM	BLGM@H	BAGM	BAGM@H	Strain Energy (Guest)	Charge Transfer (G→H)
H ₂	0.739	0.743			0.005	-0.0020
H ₂ O	0.960	0.964	HOH=105.28	HOH=103.81	0.046	0.0071
H ₂ S	1.342	1.346	SHS=92.64	SHS=92.76	0.013	-0.0029
CO	1.121	1.123			0.005	0.0004
CO ₂	1.154	1.155	OCO=180.00	OCO=178.17	0.063	0.0001
CS ₂	1.553	1.555	SCS=180.00	SCS=179.33	0.008	-0.0029
N ₂	1.087	1.087			0.001	0.0013
NO	1.137	1.138			0.003	0.0014
NO ₂	1.180	1.182	ONO=134.71	ONO=134.202	0.010	-0.0028
F ₂	1.369	1.371			0.001	0.0046
Cl ₂	2.022	2.036			0.042	-0.0268
Br ₂	2.306	2.326			0.072	-0.0409
HF	0.920	0.930			0.067	-0.0007
HCl	1.283	1.291			0.034	-0.0041
HBr	1.421	1.427			0.014	-0.0050
CH ₄	1.088	1.090	HCH=109.47	HCH=108.92	0.051	-0.0035
C ₂ H ₂	C-H=1.064 C-C=1.195	C-H=1.067 C-C=1.198	HCC=180.00	HCC=179.18	0.031	-0.0096
C ₂ H ₄	C-H=1.083 C-C=1.322	C-H=1.085 C-C=1.325	HCH=116.707	HCH=116.842	0.016	-0.0008
C ₂ H ₆	C-H=1.090 C-C=1.524	C-H=1.092 C-C=1.525	HCH=107.632	HCH=106.976	0.078	-0.0024

BLGM : Bond length of gas molecule

BAGM : Bond angle of gas molecule

BAGM@H : Bond length of gas molecule after complexation

BAGM@H : Bond angle of gas molecule after complexation

NBO charge transfer

Table S2. Gibbs free energy change (ΔG) at various temperature condition is calculated. The energy values are calculated using $\Delta G = G_{\text{pdt}} - G_{\text{rct}}$ (the difference between the product and reactant). ΔH and ΔS values are negative for all the system.

Gas Molecules	$\Delta G_{298.15}$	ΔG_{273}	ΔG_{323}	$\Delta H_{298.15}$	$\Delta S_{298.15}$
H₂	4.361	3.943		-1.309	-0.019
H₂O	0.468	-0.351		-8.864	-0.031
H₂S	0.742	-0.145		-9.388	-0.033
CO	4.428	3.616		-4.805	-0.031
CO₂	2.931	2.130		-6.180	-0.030
CS₂	-0.158		98.937	-11.081	-0.036
N₂	3.650	2.934		-4.459	-0.015
NO	5.131	4.242		-4.833	-0.033
NO₂	4.376	3.414		-6.582	-0.036
F₂	6.562	5.761		-2.546	-0.030
Cl₂	0.082	-1.315		-9.769	-0.033
Br₂	-1.325		-0.400	-12.599	-0.037
HF	-0.539		0.080	-8.133	-0.025
HCl	1.557	0.756		-7.629	-0.030
HBr	2.328	1.464		-7.530	-0.033
CH₄	4.193	3.421		-4.628	-0.029
C₂H₂	1.601	0.756		-8.022	-0.005
C₂H₄	2.226	1.357		-7.652	-0.033
C₂H₆	3.616	2.582		-8.274	-0.039

Table S3. Donor-acceptor charge transfer and their corresponding second-order perturbation stabilization energy $E^{(2)}$ of each host-guest complex.

H₂@TCC			
Host→Guest	E⁽²⁾ in kcal/mol	Guest→Host	E⁽²⁾ in kcal/mol
BD(2)C ₄₆ -C ₅₁ → BD*(1)H ₉₃ -H ₉₄	0.14		
H₂O@TCC			
BD(2)C ₇ -C ₈ → BD*(1)O ₉₃ -H ₉₅	0.25	BD(1)O ₉₃ -H ₉₄ →BD*(2)C ₁₄ -C ₁₉	0.18
BD(2)C ₉ -C ₁₀ → BD*(1)O ₉₃ -H ₉₄	0.20	LP(1)O ₉₃ →RY*(1)H ₇₁	0.16
BD(2)C ₁₄ -C ₁₉ → BD*(1)O ₉₃ -H ₉₄	0.26	LP(2)O ₉₃ →RY*(1)H ₆₇	0.20
		LP(2)O ₉₃ →RY*(1)H ₇₁	0.17
		LP(2)O ₉₃ →BD*(1)C ₂₆ -H ₇₁	0.14
H₂S@TCC			
BD(1)C ₂₇ -C ₂₈ → RY*(1)H ₉₄	0.14	LP(2)S ₉₅ →BD*(2)C ₂₉ -C ₃₀	0.16
BD(2)C ₂₇ -C ₂₈ → BD*(1)H ₉₄ -S ₉₅	0.24	LP(2)S ₉₅ →BD*(2)C ₃₃ -C ₃₄	0.16
BD(2)C ₃₃ -C ₃₄ → BD*(1)H ₉₃ -S ₉₅	0.24	LP(2)S ₉₅ →BD*(1)C ₃₉ -H ₄₀	0.20
BD(2)C ₃₇ -C ₃₈ → BD*(1)H ₉₃ -S ₉₅	0.17		
CO@TCC			
BD(2)C ₄₀ -C ₄₅ → LP*(2)C ₉₄	0.56	BD(1)O ₉₃ -C ₉₄ →RY*(3)C ₄₃	0.23
BD(2)C ₄₃ -C ₄₄ → LP*(2)C ₉₄	0.57	LP(1)C ₉₄ →BD*(2)C ₄₃ -C ₄₄	0.30
BD(2)C ₄₃ -C ₄₄ → LP*(3)C ₉₄	1.73	LP(1)C ₉₄ →BD*(2)C ₄₆ -C ₅₁	0.17
BD(2)C ₄₆ -C ₅₁ → LP*(2)C ₉₄	0.15	LP*(2)C ₉₄ →BD*(2)C ₄₀ -C ₄₅	0.19
BD(2)C ₄₆ -C ₅₁ → LP*(3)C ₉₄	1.05	LP*(2)C ₉₄ →BD*(2)C ₄₃ -C ₄₄	0.32
CO₂@TCC			
BD(2)C ₃₄ -C ₃₅ →LP*(1)C ₉₄	1.30	BD(1)O ₉₃ -C ₉₄ →RY*(1)C ₄₅	0.20
BD(2)C ₃₄ -C ₃₅ →LP*(2)C ₉₄	1.25	BD(1)C ₉₄ -O ₉₅ →RY*(1)C ₃₅	0.20
BD(2)C ₃₆ -C ₃₇ →LP*(2)C ₉₄	0.18	LP(2)O ₉₃ →BD*(2)C ₄₀ -C ₄₅	0.28
BD(2)C ₄₀ -C ₄₅ →LP*(1)C ₉₄	0.48	LP*(1)C ₉₄ →BD*(2)C ₄₃ -C ₄₄	0.18
BD(2)C ₄₀ -C ₄₅ →LP*(2)C ₉₄	2.09	LP*(2)C ₉₄ →BD*(2)C ₃₄ -C ₃₅	0.31
BD(2)C ₄₃ -C ₄₄ →LP*(1)C ₉₄	0.24	LP*(2)C ₉₄ →BD*(2)C ₃₆ -C ₃₇	0.26
		LP(2)O ₉₅ →BD*(2)C ₃₄ -C ₃₅	0.25
CS₂@TCC			
BD(2)C ₁ -C ₂ →LP(2)S ₉₅	0.42	BD(1)C ₉₃ -S ₉₄ →RY*(3)C ₅₁	0.14
BD(2)C ₁ -C ₂ →LP(3)S ₉₅	0.34		
BD(2)C ₁ -C ₂ →BD*(2)C ₉₃ -S ₉₄	0.25		
BD(2)C ₃ -C ₄ →LP(2)S ₉₅	0.99		
BD(2)C ₃ -C ₄ →LP(3)S ₉₅	15.15		
BD(2)C ₅ -C ₆ →LP(2)S ₉₅	0.88		
BD(2)C ₇ -C ₈ →LP(2)S ₉₅	1.74		
BD(2)C ₇ -C ₈ →LP(3)S ₉₅	6.57		
BD(2)C ₉ -C ₁₀ →LP(2)S ₉₅	0.41		
BD(2)C ₄₃ -C ₄₄ →BD*(3)C ₉₃ -S ₉₄	0.52		
BD(2)C ₄₆ -C ₅₁ →BD*(3)C ₉₃ -S ₉₄	0.66		
BD(2)C ₄₇ -C ₄₈ →BD*(3)C ₉₃ -S ₉₄	0.19		
N₂@TCC			
BD(1)C ₁₇ -C ₁₈ →RY*(2)N ₉₄	0.14	BD(3)N ₉₃ -N ₉₄ →RY*(3)C ₁₇	0.33
BD(2)C ₁₇ -C ₁₈ →RY*(2)N ₉₄	0.15	BD(3)N ₉₃ -N ₉₄ →RY*(3)C ₂₀	0.18
BD(2)C ₁₇ -C ₁₈ →BD*(2)N ₉₃ -N ₉₄	0.14	LP(1)N ₉₄ →BD*(2)C ₁₇ -C ₁₈	0.23
BD(1)C ₁₈ -C ₁₉ →RY*(2)N ₉₄	0.19		
BD*(2)C ₁₄ -C ₁₉ →BD*(1)N ₉₃ -N ₉₄	0.29		
BD*(2)C ₁₇ -C ₁₈ →BD*(2)N ₉₃ -N ₉₄	0.27		

NO@TCC			
		BD(2)N ₉₃ -O ₉₄ → RY*(3)C ₄₃	0.19
NO₂@TCC			
BD(1)C ₄₀ -C ₄₅ → RY*(5)N ₉₅	0.15	LP(3)O ₉₄ → BD*(2)C ₃₅ -C ₃₆	0.21
BD(1)C ₄₄ -C ₄₅ → RY*(5)N ₉₅	0.18		
BD(2)C ₄₄ -C ₄₅ → LP*(1)N ₉₅	9.82		
BD(2)C ₄₄ -C ₄₅ → LP*(2)N ₉₅	4.20		
F₂@TCC			
		BD(1)F ₉₃ -F ₉₄ → RY*(2)C ₃₅	0.14
		BD(1)F ₉₃ -F ₉₄ → RY*(2)C ₄₅	0.14
		BD(1)F ₉₃ -F ₉₄ → RY*(1)H ₇₆	0.17
		LP(3)F ₉₃ → BD*(2)C ₃₅ -C ₃₆	0.16
Cl₂@TCC			
BD(2)C ₁ -C ₂ → BD*(1)Cl ₉₃ -Cl ₉₄	1.19	LP(1)Cl ₉₃ → BD*(2)C ₁ -C ₂	0.22
BD(1)C ₂ -H ₅₇ → BD*(1)Cl ₉₃ -Cl ₉₄	0.35	LP(3)Cl ₉₃ → BD*(1)C ₁₃ -H ₆₃	0.16
BD(2)C ₃₅ -C ₃₆ → BD*(1)Cl ₉₃ -Cl ₉₄	1.19	LP(1)Cl ₉₄ → BD*(2)C ₃₅ -C ₃₆	0.22
BD(1)C ₃₅ -H ₇₆ → BD*(1)Cl ₉₃ -Cl ₉₄	0.35	LP(3)Cl ₉₄ → BD*(1)C ₃₉ -H ₇₉	0.16
BD(2)C ₄₀ -H ₄₅ → BD*(1)Cl ₉₃ -Cl ₉₄	0.21		
BD(2)C ₄₉ -H ₅₀ → BD*(1)Cl ₉₃ -Cl ₉₄	0.21		
Br₂@TCC			
BD(2)C ₉ -C ₁₀ → BD*(1)Br ₉₃ -Br ₉₄	2.06	BD(1)Br ₉₃ -Br ₉₄ → RY*(2)C ₉	0.15
BD(1)C ₉ -H ₆₀ → BD*(1)Br ₉₃ -Br ₉₄	0.35	BD(1)Br ₉₃ -Br ₉₄ → RY*(2)C ₂₈	0.15
BD(2)C ₁₄ -C ₁₉ → BD*(1)Br ₉₃ -Br ₉₄	0.15	LP(1)Br ₉₃ → BD*(2)C ₉ -C ₁₀	0.25
BD(2)C ₂₃ -C ₂₄ → BD*(1)Br ₉₃ -Br ₉₄	0.15	LP(2)Br ₉₃ → BD*(2)C ₉ -C ₁₀	0.20
BD(2)C ₂₇ -C ₂₈ → BD*(1)Br ₉₃ -Br ₉₄	2.06	LP(3)Br ₉₃ → BD*(2)C ₉ -C ₁₀	0.17
BD(2)C ₂₈ -H ₇₃ → BD*(1)Br ₉₃ -Br ₉₄	0.35	LP(3)Br ₉₃ → BD*(2)C ₁₃ -H ₆₃	0.29
		LP(1)Br ₉₄ → BD*(2)C ₂₇ -C ₂₈	0.25
		LP(2)Br ₉₄ → BD*(2)C ₂₇ -C ₂₈	0.20
		LP(3)Br ₉₄ → BD*(2)C ₂₇ -C ₂₈	0.17
		LP(3)Br ₉₄ → BD*(1)C ₃₉ -H ₇₉	0.29
HF@TCC			
BD(2)C ₄₀ -C ₄₁ LP*(1)H ₉₃	0.91	LP*(1)H ₉₃ RY*(1)C ₄₀	0.25
BD(2)C ₄₂ -C ₄₃ LP*(1)H ₉₃	6.16	LP*(1)H ₉₃ RY*(2)C ₄₁	0.38
		LP*(1)H ₉₃ RY*(3)C ₄₂	1.02
		LP*(1)H ₉₃ RY*(3)C ₄₃	1.80
		LP(3)F ₉₄ BD*(1)C ₃₅ -H ₇₆	0.23
		LP(4)F ₉₄ RY*(3)C ₄₂	0.29
		LP(4)F ₉₄ RY*(3)C ₄₃	0.64
HCl@TCC			
BD(2)C ₃₃ -C ₃₄ → BD*(1)H ₉₃ -Cl ₉₄	0.32		
BD(1)C ₃₃ -C ₃₈ → RY*(1)H ₉₃	0.14		
BD(1)C ₃₄ -C ₃₅ → RY*(1)H ₉₃	0.16		
BD(1)C ₃₅ -C ₃₆ → RY*(1)H ₉₃	0.20		
BD(2)C ₃₅ -C ₃₆ → BD*(1)H ₉₃ -Cl ₉₄	0.86		
BD(2)C ₃₇ -C ₃₈ → BD*(1)H ₉₃ -Cl ₉₄	0.29		
BD(1)C ₅₂ -H ₈₈ → RY*(1)Cl ₉₄	0.21		
HBr@TCC			
BD(1)C ₃₉ -H ₈₀ → RY*(1)Br ₉₄	0.21	BD(1)H ₉₃ -Br ₉₄ → RY*(3)C ₄₃	0.32
BD(1)C ₄₁ -C ₄₂ → RY*(1)H ₉₃	0.16		
BD(2)C ₄₁ -C ₄₂ → BD*(1)H ₉₃ -Br ₉₄	0.45		

BD(1)C ₄₂ -C ₄₃ →RY*(1)H ₉₃	0.16		
BD(2)C ₄₃ -C ₄₄ →BD*(1)H ₉₃ -Br ₉₄	1.32		
BD*(2)C ₄₃ -C ₄₄ →BD*(1)H ₉₃ -Br ₉₄	0.53		
CH₄@TCC			
BD(1)C ₂ -C ₃ →RY*(1)C ₉₃	0.20		
BD(2)C ₅ -C ₆ →BD*(1)C ₉₃ -H ₉₆	0.18		
C₂H₂@TCC			
BD(1)C ₁ -C ₂ →RY*(1)H ₉₃	0.22	BD(3)C ₉₄ -C ₉₅ →BD*(2)C ₄₃ -C ₄₄	0.14
BD(2)C ₁ -C ₂ →BD*(1)H ₉₃ -C ₉₄	0.47	BD(3)C ₉₄ -C ₉₅ →BD*(2)C ₄₆ -C ₅₁	0.14
BD(1)C ₂ -C ₃ →RY*(1)H ₉₃	0.20		
BD(1)C ₃₄ -C ₃₅ →RY*(1)H ₉₆	0.20		
BD(1)C ₃₅ -C ₃₆ →RY*(1)H ₉₆	0.22		
BD(2)C ₃₅ -C ₃₆ →BD*(1)C ₉₅ -C ₉₆	0.48		
BD(1)C ₄₄ -C ₄₅ →RY*(2)C ₉₅	0.21		
BD(1)C ₅₀ -C ₅₁ →RY*(2)C ₉₄	0.21		
C₂H₄@TCC			
BD(1)C ₃₃ -C ₃₄ →RY*(1)H ₉₇	0.14	BD(2)C ₉₄ -C ₉₅ →BD*(1)C ₃₉ -H ₈₀	0.16
BD(1)C ₄₂ -C ₄₃ →RY*(1)H ₉₃	0.14	BD(2)C ₉₄ -C ₉₅ →BD*(1)C ₅₂ -H ₈₈	0.21
C₂H₆@TCC			
BD(1)C ₂₈ -C ₂₉ RY*(1)H ₁₀₀	0.14		
BD(1)C ₃₄ -C ₃₅ RY*(1)C ₉₄	0.19		
BD(1)C ₄₄ -C ₄₅ RY*(1)C ₉₃	0.19		
BD(1)C ₅₀ -C ₅₁ RY*(1)H ₉₅	0.14		

Table S4. The electron density $\rho(r_c)$, Laplacian electron density $\nabla^2\rho(r_c)$, kinetic energy $G(r_c)$, potential energy $V(r_c)$, total energy density $H(r_c)$ and the ratio of potential and kinetic energy density.

Carbazole	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1...H2	0.0000059	-0.0000059	0.0000036	-0.0000013	0.0000023	0.3523040
H3...H4	0.0000059	-0.0000059	0.0000036	-0.0000013	0.0000023	0.3523040

H ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1...H2	0.0000045	-0.0000054	0.0000033	-0.0000012	0.0000020	0.3772460
C4...H2	0.0058620	-0.0051860	0.0042700	-0.0033540	0.0009160	0.7854800
C5...H3	0.0075350	-0.0058270	0.0050310	-0.0042360	0.0007950	0.8419800
H6...H1	0.0000050	-0.0000057	0.0000035	-0.0000013	0.0000022	0.3749650

H ₂ O	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1...O2	0.0000636	-0.0001000	0.0000577	-0.0000148	0.0000429	0.2562770
H5...O2	0.0036880	-0.0031810	0.0026630	-0.0021450	0.0005180	0.8054825
C8...H3	0.0095830	-0.0077350	0.0065410	-0.0053470	0.0011940	0.8174591
C6...H4	0.0085180	-0.0069930	0.0059110	-0.0048290	0.0010820	0.8169514
C7...H4	0.0080500	-0.0064490	0.0054790	-0.0045090	0.0009700	0.8229603
H9...H10	0.0000048	-0.0000049	0.0000030	-0.0000012	0.0000018	0.3911342

H ₂ S	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1...S2	0.0000340	-0.0000250	0.0000160	-0.0000080	0.0000080	0.5000000
H5...S2	0.0014230	-0.0010960	0.0007910	-0.0004850	0.0003060	0.6131479
H6...S2	0.0013380	-0.0010610	0.0007620	-0.0004620	0.0003000	0.6062992
H8...S2	0.0042150	-0.0031090	0.0025020	-0.0018960	0.0006060	0.7577937
C7...H3	0.0084490	-0.0065050	0.0055100	-0.0045160	0.0009940	0.8196007
C9...H4	0.0088220	-0.0068190	0.0057850	-0.0047510	0.0010340	0.8212618

CO	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1...C3	0.0000039	-0.0000061	0.0000037	-0.0000012	0.0000025	0.3243243
H1...H8	0.0000030	-0.0000030	0.0000022	-0.0000008	0.0000014	0.3684210
O2...H4	0.0014350	-0.0015560	0.0011590	-0.0007620	0.0003970	0.6574633
O2...H6	0.0025330	-0.0024160	0.0018950	-0.0013730	0.0005220	0.7245382
O2...H5	0.0001980	-0.0002480	0.0001503	-0.0000521	0.0000982	0.3466400
C3...C7	0.0102040	-0.0083460	0.0070450	-0.0057450	0.0013000	0.8154719

CO ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1...O2	0.0000310	-0.0000530	0.0000311	-0.0000086	0.0000225	0.2768154
H4...O3	0.0038750	-0.0032810	0.0027900	-0.0022990	0.0004910	0.8240143
H5...O3	0.0000310	-0.0000537	0.0000311	-0.0000086	0.0000225	0.2757647
H6...O2	0.0038770	-0.0032820	0.0027910	-0.0023000	0.0004910	0.8240773
C7...O2	0.0077610	-0.0068470	0.0056250	-0.0044030	0.0012220	0.7827555
C8...O3	0.0077590	-0.0068450	0.0056230	-0.0044020	0.0012210	0.7828561

CS ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	G(r_c)	V(r_c)	H(r_c)	V(r_c)/ G(r_c)
H1...S2	0.0007280	-0.0005610	0.0003850	-0.0002080	0.0001770	0.5402597
H5...S3	0.0007280	-0.0005610	0.0003840	-0.0002080	0.0001760	0.5416666
H6...C4	0.0030530	-0.0023110	0.0018680	-0.0014260	0.0004420	0.7633832
H7...C4	0.0030490	-0.0023080	0.0018660	-0.0014230	0.0004430	0.7625937
C8...S3	0.0085240	-0.0066410	0.0056150	-0.0045880	0.0010270	0.8170970
C9...S2	0.0085220	-0.0066380	0.0056130	-0.0045880	0.0010250	0.8173882

N ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	G(r_c)	V(r_c)	H(r_c)	V(r_c)/ G(r_c)
H1...N3	0.0001760	-0.0002260	0.0001390	-5.3292490	0.0000532	0.3833812
H6...N3	0.0017410	-0.0015690	0.0012050	-0.0008400	0.0003650	0.6970954
H7...N3	0.0034530	-0.0029730	0.0023620	-0.0017500	0.0006120	0.7408975
C8...N2	0.0093060	-0.0085330	0.0070770	-0.0056220	0.0014550	0.7944044
H4...H5	0.0000030	-0.00000330	0.0000020	-0.0000008	0.0000012	0.3932038

NO	$\rho(r_c)$	$\nabla^2\rho(r_c)$	G(r_c)	V(r_c)	H(r_c)	V(r_c)/ G(r_c)
H1...O2	0.0019210	-0.0017290	0.0012820	-0.0008340	0.0004480	0.6505460
H4...O2	0.0050100	-0.0050220	0.0038530	-0.0026850	0.0011680	0.6968595
C5...N3	0.0119570	-0.0103500	0.0091020	-0.0078540	0.0012480	0.8628872
H6...N3	0.0000040	-0.0000060	0.0000036	-0.0000012	0.0000024	0.3433242
H7...H6	0.0000040	-0.0000044	0.0000027	-0.0000009	0.0000017	0.3670370

NO ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	G(r_c)	V(r_c)	H(r_c)	V(r_c)/ G(r_c)
H1...O3	0.0000220	-0.0000506	0.0000294	-0.0000081	0.0000215	0.2772108
H5...N2	0.0035270	-0.0030800	0.0025870	-0.0020930	0.0004940	0.8090452
H6...N4	0.0000210	-0.0000393	0.0000228	-0.0000064	0.0000169	0.2795980
H7...O3	0.0043390	-0.0035470	0.0030600	-0.0025740	0.0004860	0.8411764
C8...O3	0.0073540	-0.0061730	0.0053710	-0.0045700	0.0008010	0.8508657
C9...N2	0.0105800	-0.0087630	0.0073490	-0.0059350	0.0014140	0.8075928
H4...O4	0.0000210	-0.0000393	0.0000228	-0.0000064	0.0000164	0.2799475

F ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	G(r_c)	V(r_c)	H(r_c)	V(r_c)/ G(r_c)
H1...F2	0.0000040	-0.0000115	0.0000066	-0.0000017	0.0000048	0.2665662
H4...F3	0.0015450	-0.0020200	0.0014880	-0.0009550	0.0005330	0.6418010
H5...F3	0.0000100	-0.0000238	0.0000136	-0.0000035	0.0000101	0.2593404
H6...F2	0.0014960	-0.0019240	0.0014170	-0.0009110	0.0005060	0.6429075
C7...F3	0.0070690	-0.0069020	0.0060240	-0.0051470	0.0008770	0.8544156
C8...F2	0.0067580	-0.0063160	0.0055400	-0.0047650	0.0007750	0.8601083
H1...H6	0.0000040	-0.0000044	0.0000027	-0.0000011	0.0000016	0.4000000
H4...H5	0.0000040	-0.0000047	0.0000029	-0.0000011	0.0000017	0.3862234

Cl ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	G(r_c)	V(r_c)	H(r_c)	V(r_c)/ G(r_c)
H1...Cl2	0.0000150	-0.0000181	0.0000115	-0.0000049	0.0000065	0.4313043
H1...Cl3	0.0000150	-0.0000181	0.0000115	-0.0000049	0.0000065	0.4299956
H4...Cl2	0.0048780	-0.0037410	0.0030010	-0.0022610	0.0007400	0.7534155
H5...Cl3	0.0048780	-0.0037410	0.0030010	-0.0022610	0.0007400	0.7534155
C6...Cl2	0.0079890	-0.0065040	0.0053190	-0.0041340	0.0011850	0.7772137
C7...Cl3	0.0079880	-0.0065030	0.0053180	-0.0041330	0.0011850	0.7771718
C8...Cl2	0.0085560	-0.0076090	0.0061970	-0.0047840	0.0014130	0.7719864
C9...Cl3	0.0085580	-0.0076110	0.0061980	-0.0047850	0.0014130	0.7720232

Br ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1 $\cdots$ Br2	0.0000370	-0.0000393	0.0000249	-0.0000105	0.0000249	0.0000144
H1 $\cdots$ Br3	0.0000370	-0.0000393	0.0000249	-0.0000105	0.0000249	0.0000143
H4 $\cdots$ Br2	0.0055630	-0.0039910	0.0032860	-0.0025820	0.0032860	0.0007040
H5 $\cdots$ Br3	0.0055630	-0.0039900	0.0032860	-0.0025810	0.0032860	0.0007050
C6 $\cdots$ Br2	0.0084810	-0.0063190	0.0052970	-0.0042760	0.0052970	0.0010210
C7 $\cdots$ Br3	0.0084810	-0.0063180	0.0052970	-0.0042760	0.0052970	0.0010210
C8 $\cdots$ Br2	0.0107670	-0.0082120	0.0070210	-0.0058310	0.0070210	0.0011900
C9 $\cdots$ Br3	0.0107680	-0.0082120	0.0070220	-0.0058310	0.0070220	0.0011910

HF	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1 $\cdots$ F2	0.0000610	-0.0000784	0.0000486	-0.0000188	0.0000297	0.3877055
H4 $\cdots$ F2	0.0026680	-0.0026910	0.0020580	-0.0014250	0.0006330	0.6924198
H5 $\cdots$ F2	0.0062460	-0.0062700	0.0049580	-0.0036470	0.0013110	0.7355788
C6 $\cdots$ H3	0.0147680	-0.0113540	0.0098360	-0.0083180	0.0015180	0.8456689
H7 $\cdots$ H8	0.0000050	-0.0000059	0.0000036	-0.0000013	0.0000022	0.3765753

HCl	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1 $\cdots$ Cl2	0.0006218	-0.0004940	0.0003490	-0.0002050	0.0001440	0.5873925
H4 $\cdots$ Cl2	0.0022970	-0.0017410	0.0013330	-0.0009240	0.0004090	0.6931732
C5 $\cdots$ Cl2	0.0033050	-0.0024690	0.0019080	-0.0013460	0.0005620	0.7054507
H6 $\cdots$ Cl2	0.0000094	-0.0000121	0.0000074	-0.0000028	0.0000046	0.3782951
C7 $\cdots$ H3	0.0139260	-0.0102100	0.0090370	-0.0078630	0.0011741	0.8700896

HBr	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1 $\cdots$ Br2	0.0009010	-0.0006890	0.0004980	-0.0003080	0.0001900	0.6184738
H4 $\cdots$ Br2	0.0000190	-0.0000204	0.0000129	-0.0000054	0.0000075	0.4199783
H5 $\cdots$ Br2	0.0036550	-0.0028370	0.0022910	-0.0017460	0.0005450	0.7621126
H6 $\cdots$ Br2	0.0027330	-0.0018910	0.0014940	-0.0010970	0.0003970	0.7342704
C7 $\cdots$ Br2	0.0034720	-0.0023190	0.0018440	-0.0013690	0.0004750	0.7424078
C8 $\cdots$ H3	0.0127140	-0.0094580	0.0080840	-0.0067100	0.0013740	0.8300346

CH ₄	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1 $\cdots$ H3	0.0000110	-0.0000137	0.0000084	-0.0000031	0.0000053	0.3720379
H2 $\cdots$ H8	0.0003600	-0.0003480	0.0002260	-0.0001030	0.0001230	0.4557522
H2 $\cdots$ H9	0.0017360	-0.0014490	0.0011100	-0.0007700	0.0003400	0.6936936
H4 $\cdots$ C10	0.0039520	-0.0032290	0.0025950	-0.0019610	0.0006340	0.7556840
H5 $\cdots$ C7	0.0064740	-0.0049520	0.0043020	-0.0036520	0.0006500	0.8489074
C6 $\cdots$ C11	0.0068070	-0.0059480	0.0048730	-0.0037990	0.0010740	0.7796018

C ₂ H ₂	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$ V(r_c)/G(r_c) $
H1 $\cdots$ (C $\equiv$ C)	0.0000150	0.0000210	0.0000124	-0.0000037	0.0000087	0.2980259
H2 $\cdots$ C6	0.0065220	-0.0045490	0.0038210	-0.0030930	0.0007280	0.8094739
H5 $\cdots$ C7	0.0064760	-0.0045140	0.0037940	-0.0030730	0.0007210	0.8099631
C8 $\cdots$ C3	0.0073270	-0.0055540	0.0046160	-0.0036780	0.0009380	0.7967937
C9 $\cdots$ C4	0.0073400	-0.005580	0.0046350	-0.0036900	0.0009450	0.7961165
H10 $\cdots$ (C $\equiv$ C)	0.0045360	-0.0032140	0.0027200	-0.0022270	0.0004930	0.8187500

C₂H₄	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$V(r_c)/G(r_c)$
H1...H2	0.0002850	-0.0002740	0.0001733	-0.0000720	0.0001012	0.4155155
H12...H2	0.0002470	-0.0002570	0.0001681	-0.0000783	0.0000898	0.4657387
H13...H3	0.0003070	-0.0002950	0.0001872	-0.0000792	0.0001079	0.4232843
C9...H4	0.0084280	-0.0067130	0.0056390	-0.0045650	0.0010740	0.8095406
C10...C5	0.0080730	-0.0061830	0.0052240	-0.0042650	0.0009590	0.8164241
H8...C7	0.0044850	-0.0025610	0.0022400	-0.0019200	0.0003200	0.8571428
H11...C7	0.0038180	-0.0022030	0.0019140	-0.0016240	0.0002900	0.8484848

C₂H₆	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$V(r_c)/G(r_c)$
H1...H3	0.0003250	-0.0003060	0.0001950	-0.0000850	0.0001100	0.4358974
H2...C10	0.0073070	-0.0059180	0.0050660	-0.0042150	0.0008510	0.8320173
H4...H12	0.0003240	-0.0003050	0.0001950	-0.0000850	0.0001100	0.4358974
H5...C9	0.0073300	-0.0059250	0.0050770	-0.0042290	0.0008480	0.8329722
H6...C11	0.0061470	-0.0046370	0.0039170	-0.0031960	0.0007210	0.8159305
H7...C8	0.0061190	-0.0046170	0.0039000	-0.0031840	0.0007160	0.8164102

Table S5. Energy decomposition analysis of TCC encapsulated guest molecules. The energy components are such as Electrostatic, Exchange, Dispersion, Induction (A $\leftarrow$ B/ B $\leftarrow$ A) terms are expressed in kcal/mol.

Complexes	Electrostatic	Exchange	Dispersion	Induction (A$\leftarrow$B)	Induction (B$\leftarrow$A)
H₂@TCC	-1.644	3.647	-2.547	-0.247	-0.148
H₂O@TCC	-7.094	8.844	-5.224	-1.651	-0.153
H₂S@TCC	-7.988	12.135	-9.754	-1.312	-0.356
CO@TCC	-4.751	8.860	-6.875	-0.750	-0.374
CO₂@TCC	-5.343	9.749	-7.757	-0.905	-0.173
CS₂@TCC	-9.082	18.504	-18.750	-0.812	-0.793
N₂@TCC	-3.592	7.772	-6.653	-0.290	-0.438
NO@TCC	-9.771	9.287	-6.180	-30.574	-0.102
NO₂@TCC	-10.128	10.496	-9.035	-69.012	-0.345
F₂@TCC	-2.243	5.818	-3.061	-0.291	-0.112
Cl₂@TCC	-8.422	17.686	-12.682	-1.873	-0.682
Br₂@TCC	-12.582	24.349	-17.256	-3.329	-0.647
HF@TCC	-6.440	7.513	-3.224	-2.978	-0.146
HCl@TCC	-5.806	9.768	-7.061	-2.366	-0.224
HBr@TCC	-6.479	11.325	-8.874	-2.091	-0.308
CH₄@TCC	-3.082	7.671	-7.310	-0.222	-0.405
C₂H₂@TCC	-7.685	13.620	-10.979	-1.573	-0.321
C₂H₄@TCC	-6.595	12.216	-11.094	-0.695	-0.486
C₂H₆@TCC	-4.898	12.761	-12.981	-0.322	-0.728

Figure S1. Optimized geometry of $n\text{C}_2\text{H}_6@\text{TCC}$ ($n=2,3,4$) and the corresponding C_2H_6 cluster

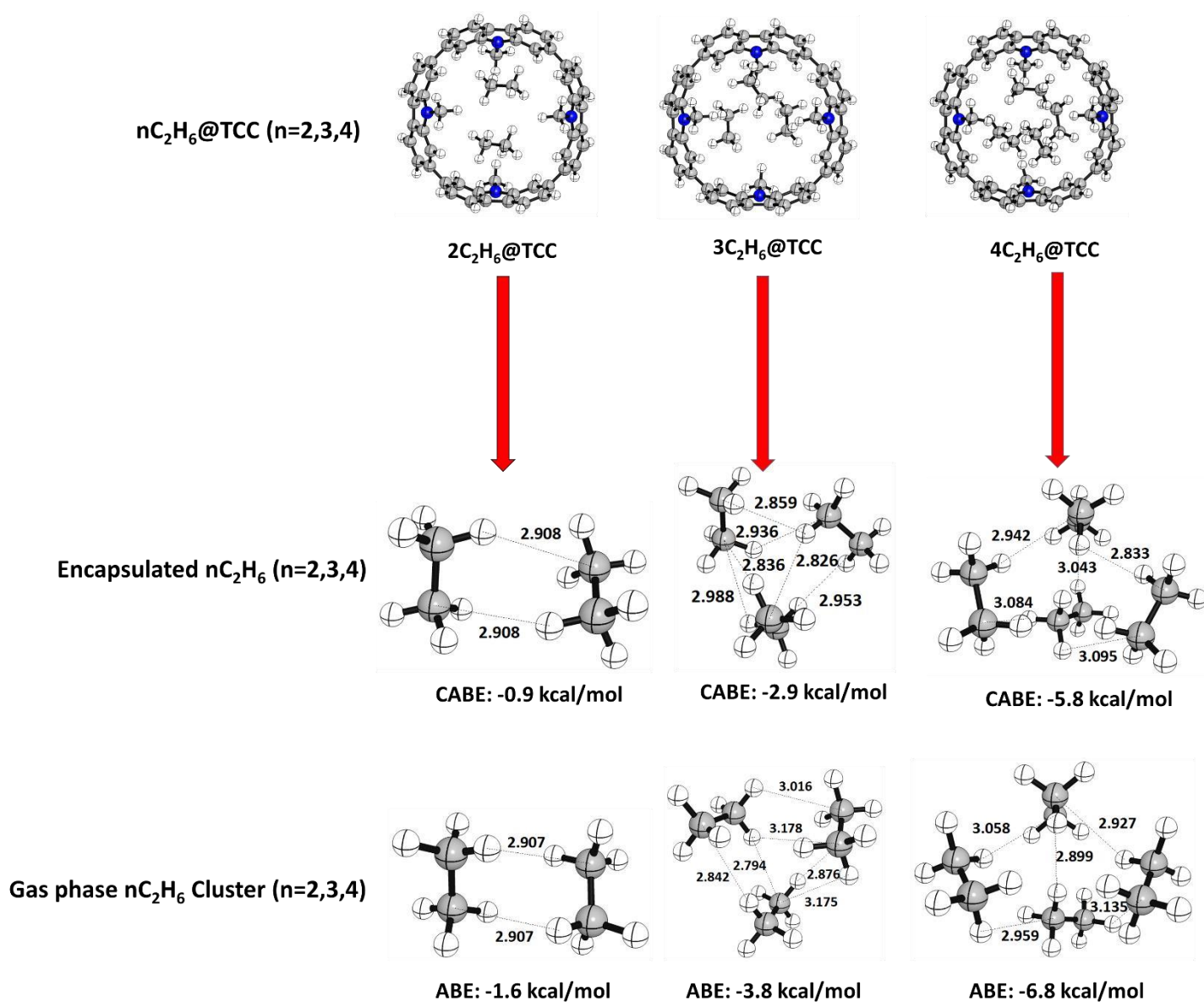


Figure S2. The molecular electrostatic surface potential plot of each TCC encapsulated guest molecules with an isosurface value of 0.02.

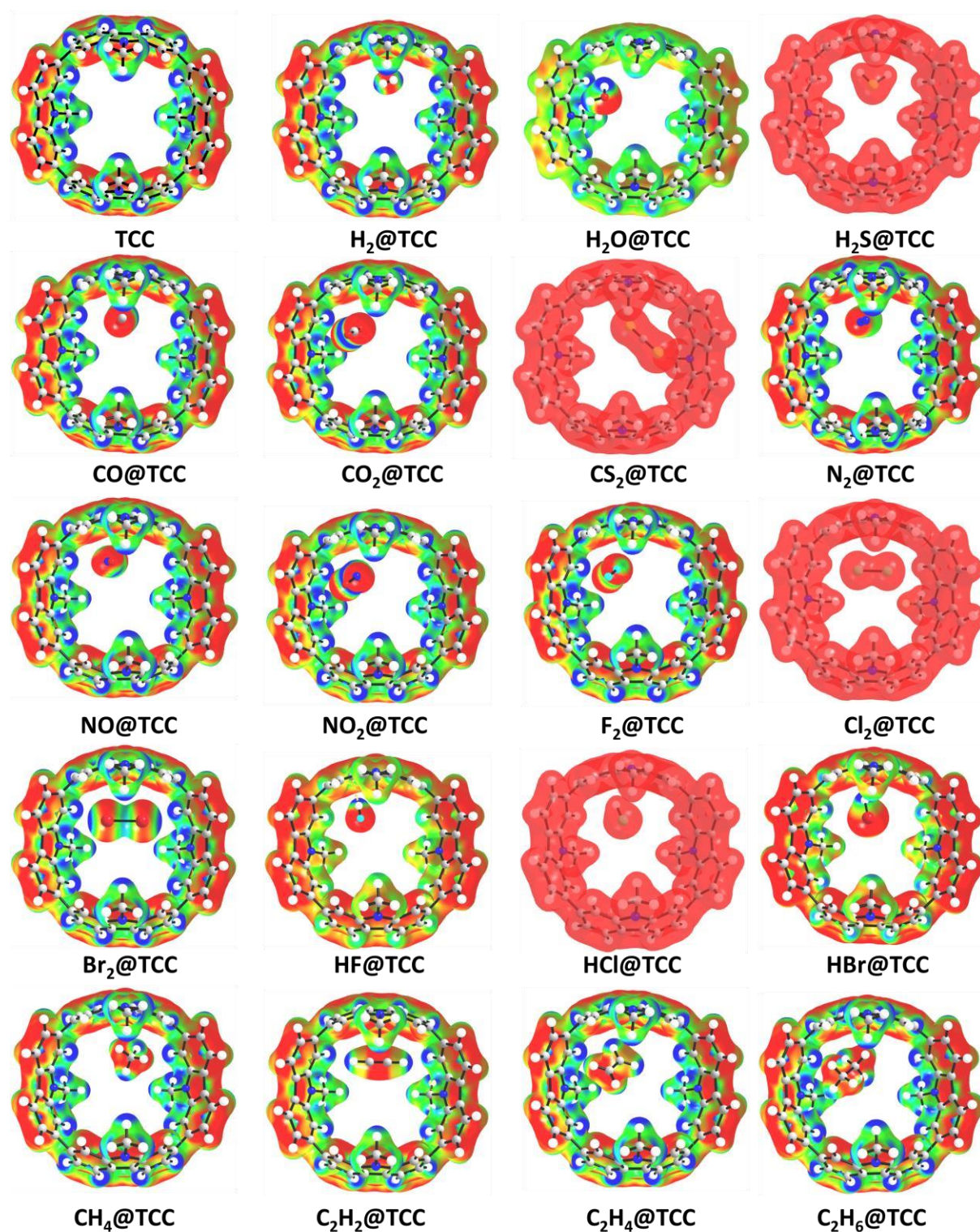


Figure S3. Atoms in molecule analysis of gas entrapped TCC complex. The red dots are expressed as the bond critical point.

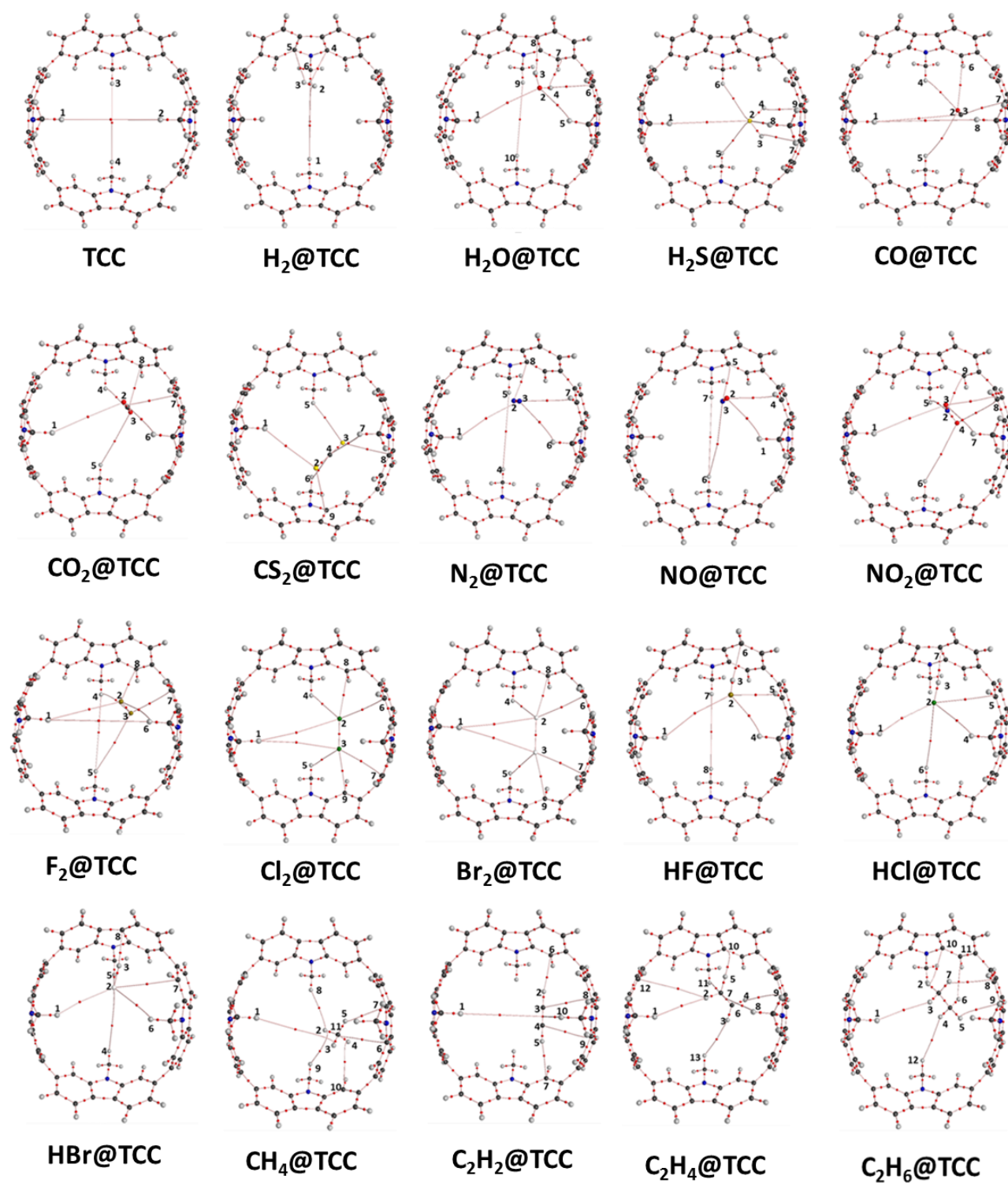


Figure S4. The NCI RDG S vs $\text{sign}(\lambda_2)\rho$ plots for guest@TCC complexes merged with TCC host. The green and red plot represent TCC and guest@TCC complex.

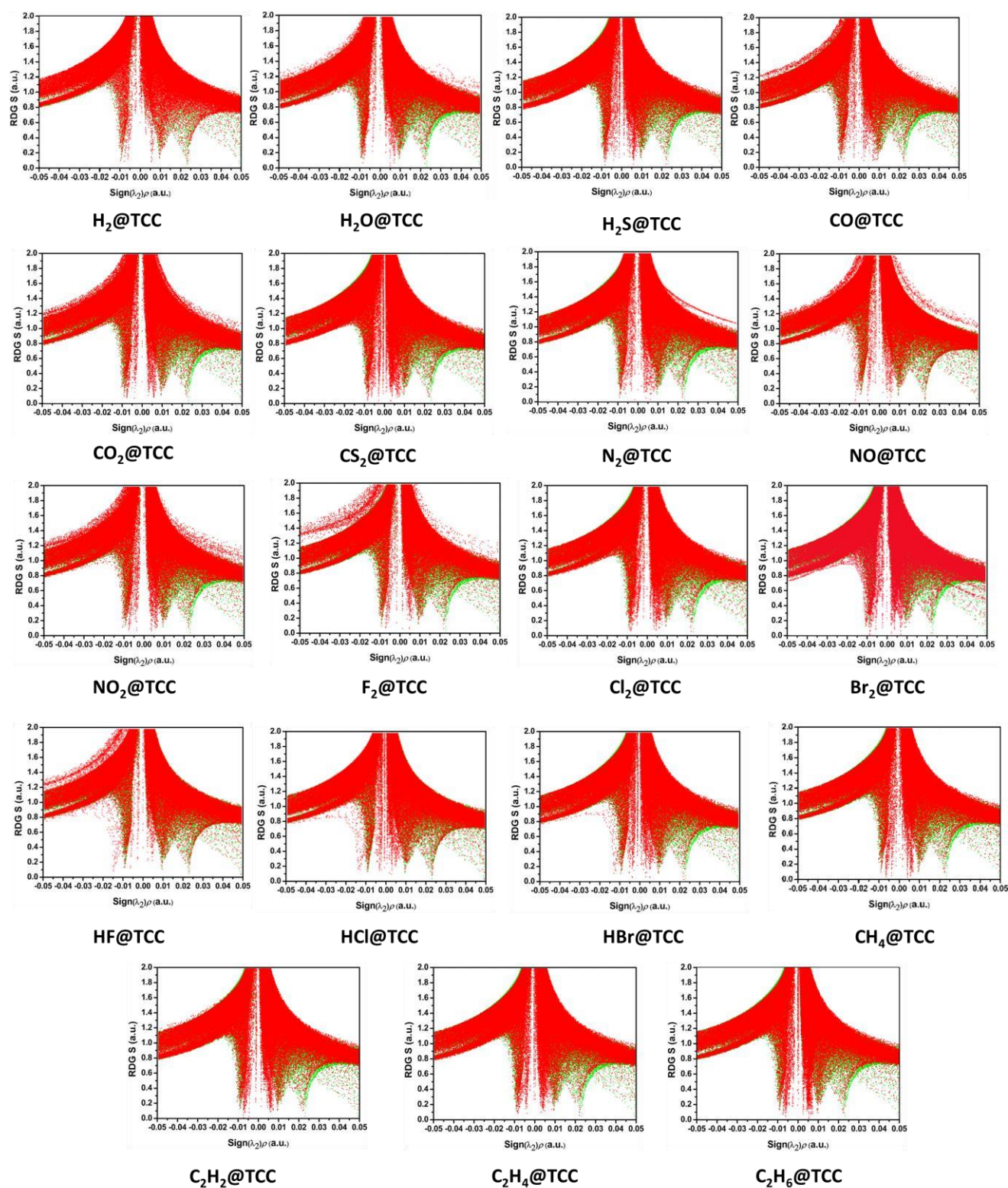


Figure S5. The interaction energy of each guest molecule with the different functional sites of TCC molecule.

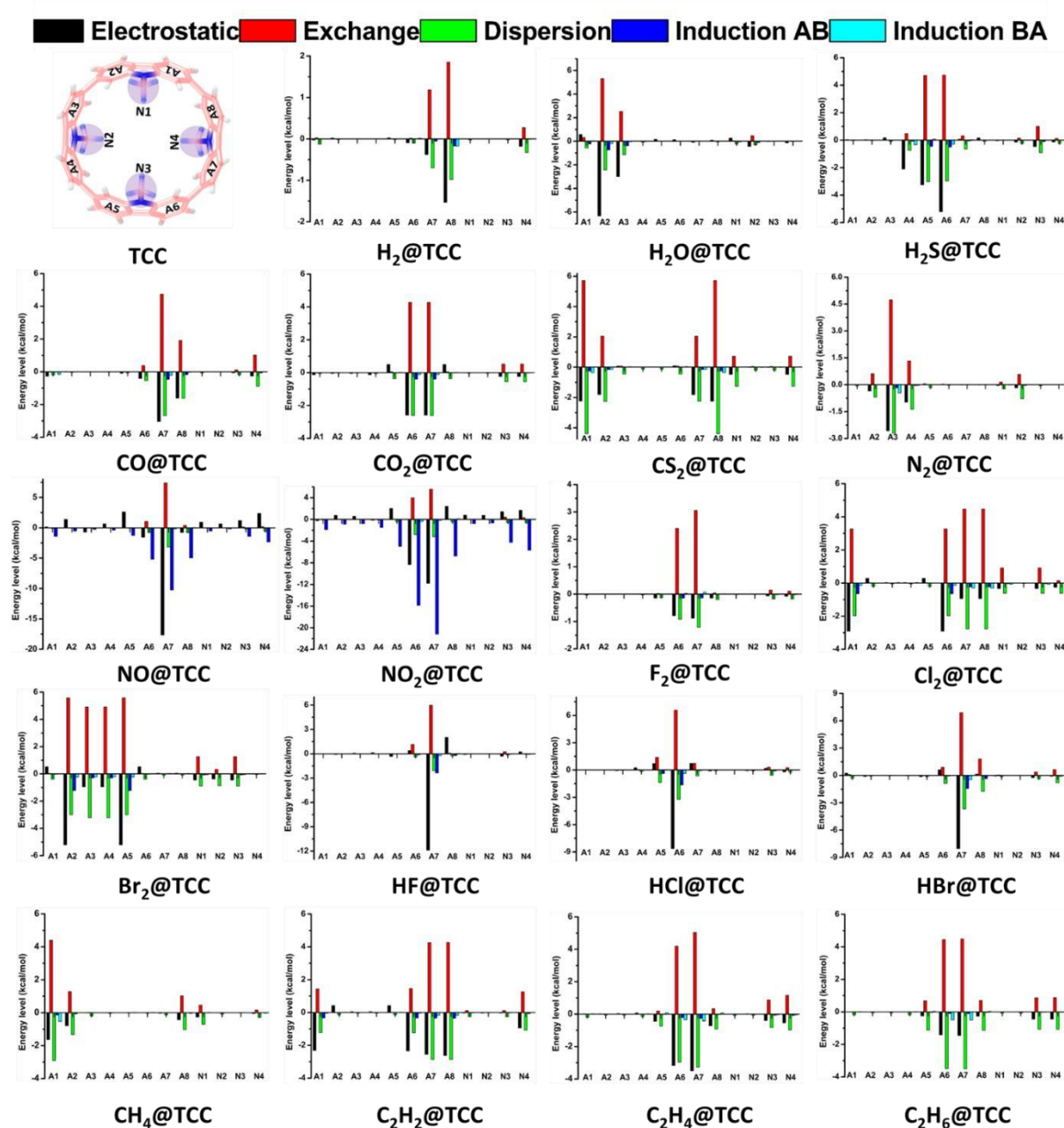


Figure S6. Correlation between the F-SAPT0 energy terms with the binding energy.

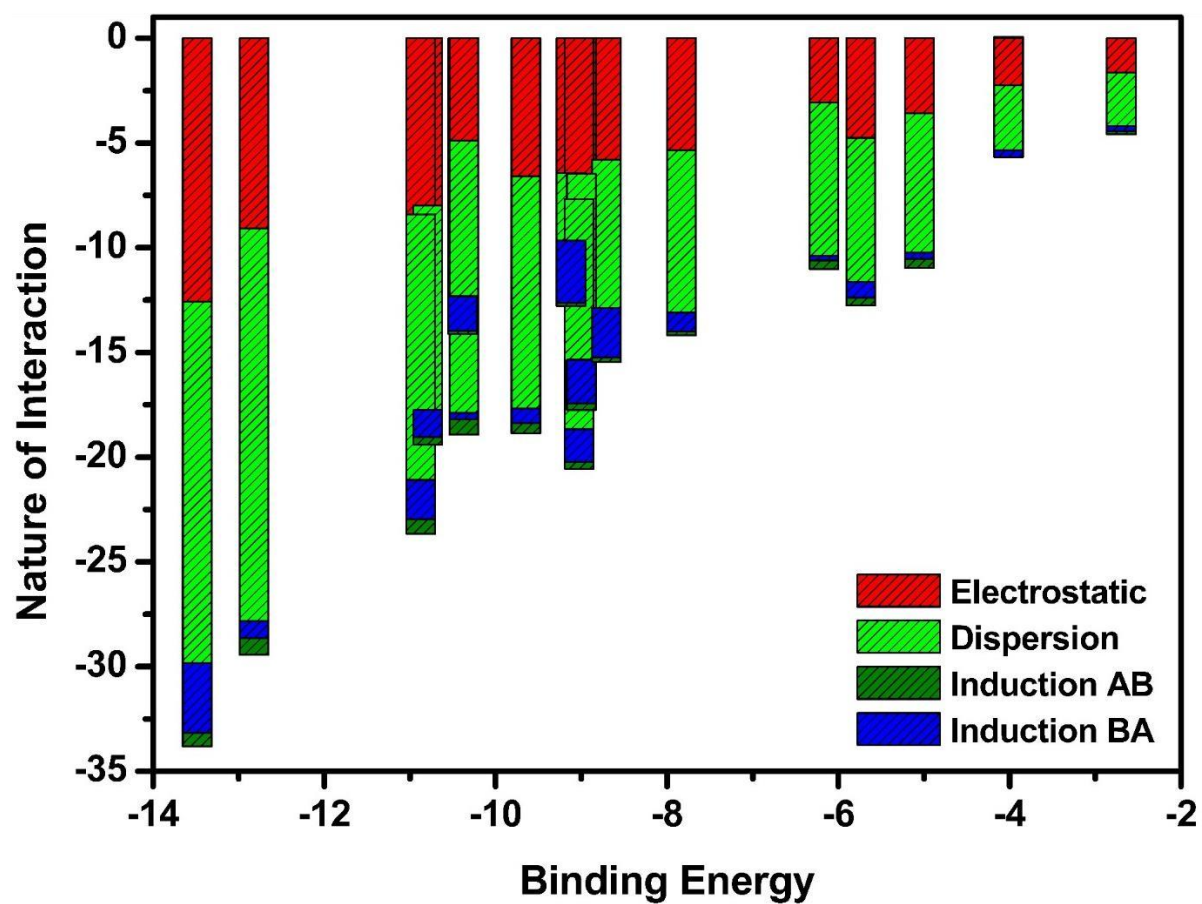


Figure S7. GCMC simulation of each gas molecule at 77, 273, 298 K temperature and pressure up to 100 bar.

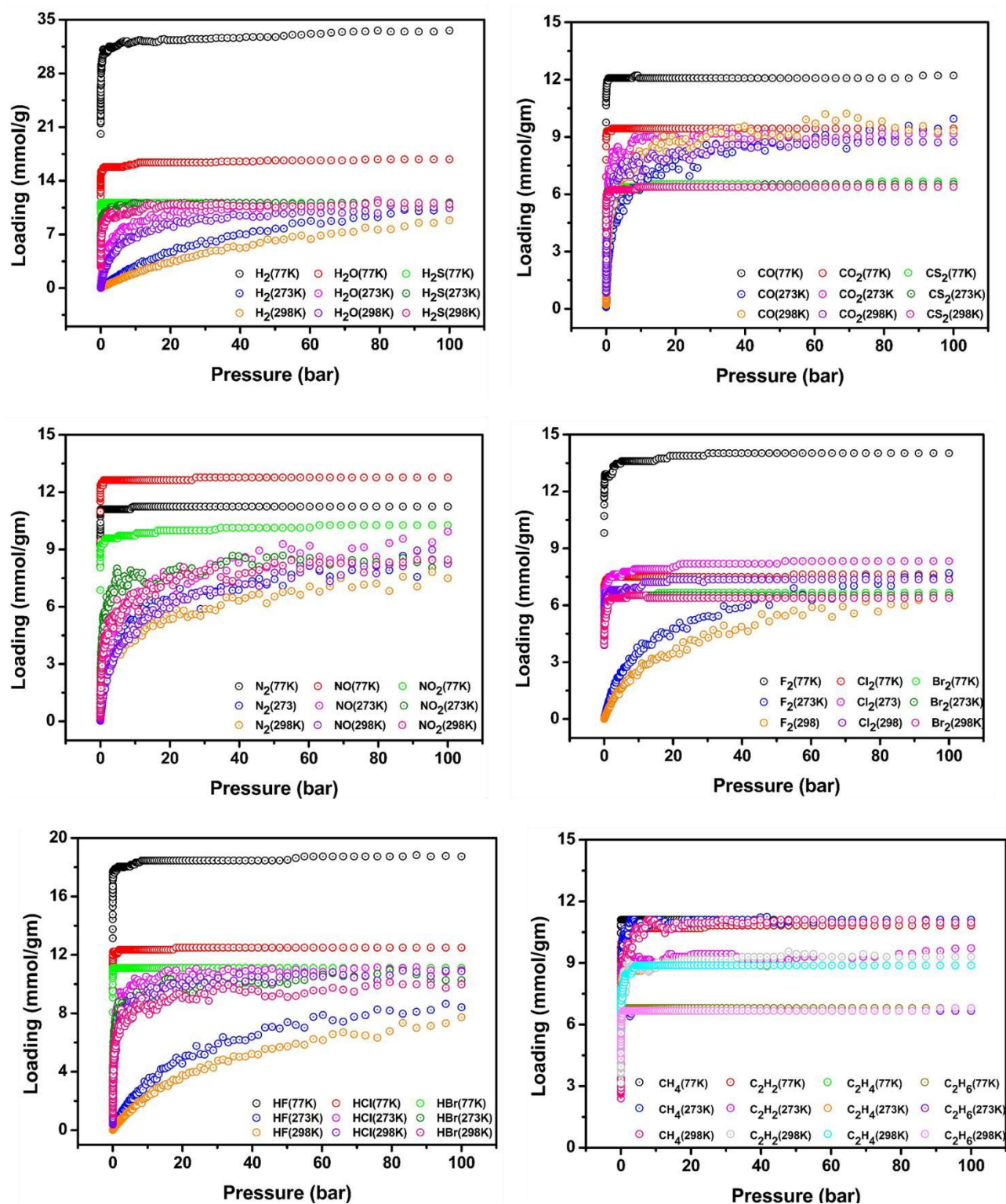
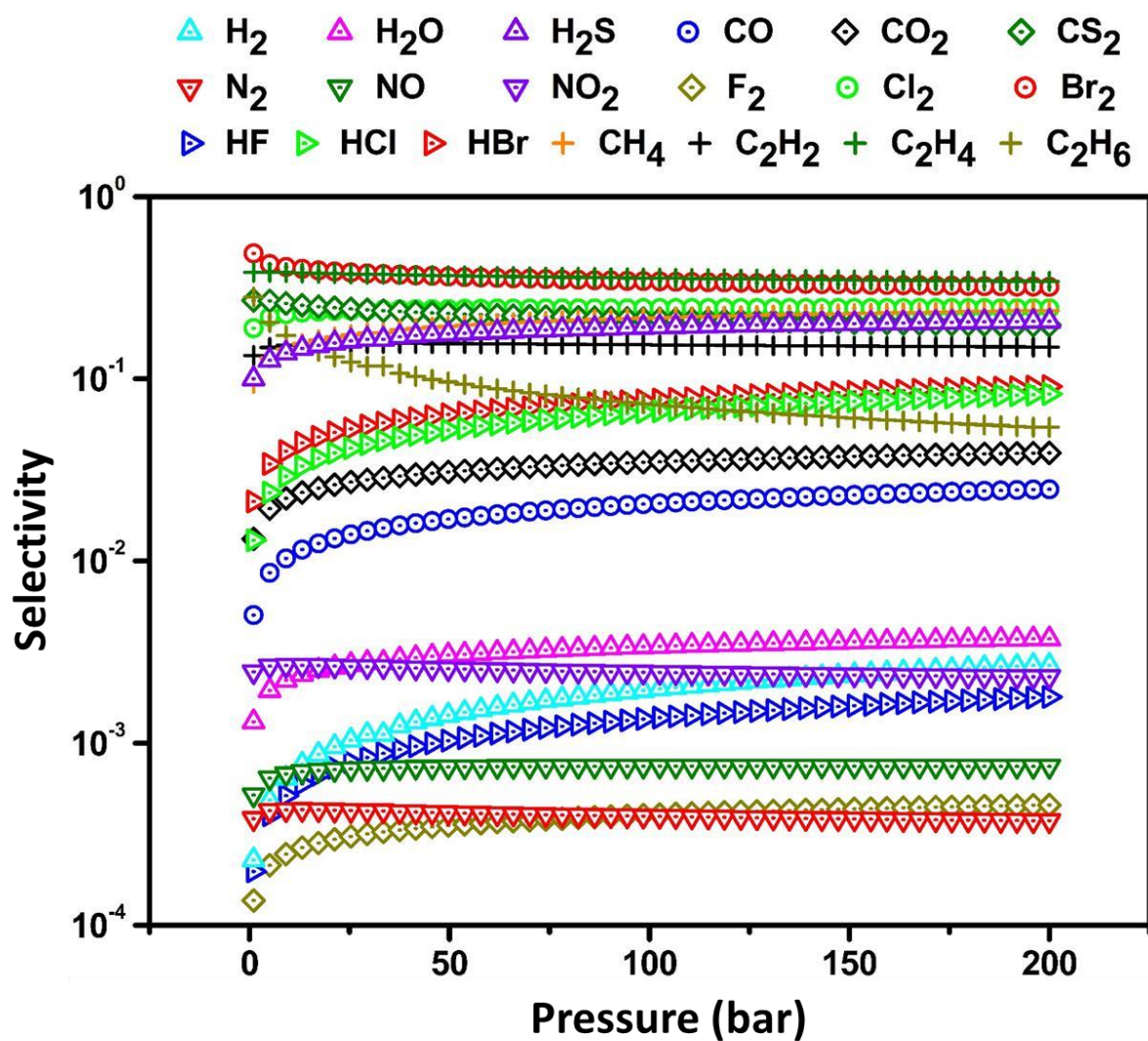


Figure S8. Selectivity of all the gas molecules at 298K temperature by using dual site Langmuir adsorption isotherm.



Coordinates of the optimized structure at the M062X-D3/TZVP level of theory.

TCC

C	-5.176809000	-1.690224000	0.027428000
C	-4.872669000	-0.848094000	-1.037996000
C	-4.949549000	0.525403000	-0.841812000
C	-5.345496000	1.081870000	0.392001000
C	-5.811980000	0.223728000	1.389539000
C	-5.722525000	-1.146118000	1.205610000
C	-4.872786000	2.453503000	0.385651000
C	-4.219750000	2.637224000	-0.850899000
C	-3.310337000	3.667480000	-1.056007000
C	-3.030121000	4.527166000	0.001809000
C	-3.797747000	4.448659000	1.179420000
C	-4.711464000	3.426449000	1.373869000
C	-3.660360000	1.252059000	-2.850285000
C	-1.690174000	5.176637000	-0.027466000
C	-1.146070000	5.722469000	-1.205604000
C	0.223724000	5.811825000	-1.389600000
C	1.081899000	5.345442000	-0.392037000
C	0.525433000	4.949452000	0.841763000
C	-0.848058000	4.872529000	1.037955000
C	2.453540000	4.872755000	-0.385670000
C	3.426509000	4.711460000	-1.373873000
C	4.448665000	3.797724000	-1.179455000
C	4.527192000	3.030091000	-0.001845000
C	3.667511000	3.310285000	1.055971000
C	2.637233000	4.219673000	0.850851000
C	1.252161000	3.660475000	2.850337000
C	5.176745000	1.690184000	0.027468000
C	4.872758000	0.848053000	-1.037988000
C	4.949584000	-0.525439000	-0.841781000
C	5.345434000	-1.081912000	0.392066000
C	5.811832000	-0.223766000	1.389641000
C	5.722360000	1.146084000	1.205702000
C	4.872774000	-2.453564000	0.385652000
C	4.219733000	-2.637245000	-0.850897000
C	3.310286000	-3.667476000	-1.056009000
C	3.030139000	-4.527242000	0.001771000
C	3.797775000	-4.448761000	1.179373000
C	4.711466000	-3.426539000	1.373843000
C	3.660440000	-1.252072000	-2.850301000
C	1.690207000	-5.176694000	-0.027474000
C	1.146091000	-5.722441000	-1.205627000
C	-0.223758000	-5.811881000	-1.389551000
C	-1.081873000	-5.345337000	-0.392033000
C	-0.525373000	-4.949381000	0.841775000
C	0.848118000	-4.872593000	1.037973000
C	-2.453526000	-4.872676000	-0.385640000
C	-3.426552000	-4.711499000	-1.373789000
C	-4.448795000	-3.797823000	-1.179333000
C	-4.527244000	-3.030103000	-0.001792000
C	-3.667506000	-3.310206000	1.056004000

C	-2.637212000	-4.219568000	0.850884000
C	-1.252066000	-3.660286000	2.850341000
N	-4.400421000	1.514275000	-1.640726000
N	1.514317000	4.400393000	1.640686000
N	4.400457000	-1.514299000	-1.640716000
N	-1.514240000	-4.400231000	1.640701000
H	-4.392469000	-1.252892000	-1.919612000
H	-6.157401000	0.619522000	2.337071000
H	-5.993992000	-1.813850000	2.014247000
H	-2.680742000	3.678907000	-1.936561000
H	-3.600412000	5.150411000	1.980670000
H	-5.227418000	3.336080000	2.322286000
H	-2.647434000	0.893995000	-2.636617000
H	-3.599945000	2.164302000	-3.441357000
H	-1.813837000	5.994259000	-2.014107000
H	0.619510000	6.157159000	-2.337170000
H	-1.252854000	4.392323000	1.919573000
H	3.336211000	5.227546000	-2.322229000
H	5.150664000	3.600675000	-1.980557000
H	3.678988000	2.680713000	1.936546000
H	0.894168000	2.647495000	2.636816000
H	4.392627000	1.252842000	-1.919645000
H	6.157160000	-0.619553000	2.337210000
H	5.993731000	1.813827000	2.014368000
H	2.680668000	-3.678882000	-1.936549000
H	3.600475000	-5.150545000	1.980598000
H	5.227443000	-3.336199000	2.322250000
H	2.647484000	-0.894075000	-2.636665000
H	3.600098000	-2.164293000	-3.441415000
H	1.813810000	-5.993952000	-2.014266000
H	-0.619562000	-6.157291000	-2.337085000
H	1.252944000	-4.392410000	1.919585000
H	-3.336212000	-5.227502000	-2.322182000
H	-5.150617000	-3.600606000	-1.980552000
H	-3.678930000	-2.680561000	1.936522000
H	-2.164300000	-3.600012000	3.441442000
H	-0.503732000	-4.187712000	3.439521000
H	-0.894103000	-2.647303000	2.636778000
H	0.503854000	4.187942000	3.439518000
H	4.187861000	-0.503750000	-3.439501000
H	-4.187793000	0.503788000	-3.439540000
H	2.164419000	3.600203000	3.441405000

H₂@TCC

C	-3.730875000	3.948192000	0.025529000
C	-2.834435000	4.019609000	-1.036912000
C	-1.622949000	4.671038000	-0.840978000
C	-1.290253000	5.274195000	0.389534000
C	-2.267762000	5.339582000	1.383907000
C	-3.471548000	4.679375000	1.200016000
C	0.152010000	5.431744000	0.383825000
C	0.597922000	4.912380000	-0.849536000
C	1.919565000	4.535516000	-1.053115000
C	2.817178000	4.660475000	0.003132000
C	2.415854000	5.324624000	1.177724000

C	1.099796000	5.710335000	1.370111000
C	-0.416552000	3.794473000	-2.838329000
C	3.982707000	3.733609000	-0.025469000
C	4.708485000	3.476904000	-1.204053000
C	5.377344000	2.278186000	-1.388525000
C	5.326076000	1.303516000	-0.390484000
C	4.732074000	1.636554000	0.844319000
C	4.072752000	2.843775000	1.040911000
C	5.485106000	-0.138497000	-0.384986000
C	5.751646000	-1.086182000	-1.374769000
C	5.359523000	-2.400120000	-1.181604000
C	4.700530000	-2.798992000	-0.003190000
C	4.591917000	-1.903661000	1.056696000
C	4.975591000	-0.583924000	0.852540000
C	3.878345000	0.429427000	2.852161000
C	3.759698000	-3.953337000	0.025390000
C	2.864249000	-4.027016000	-1.037636000
C	1.651628000	-4.675912000	-0.840755000
C	1.317701000	-5.275711000	0.391018000
C	2.295017000	-5.341036000	1.385696000
C	3.499516000	-4.682470000	1.201047000
C	-0.125057000	-5.428558000	0.386636000
C	-0.570112000	-4.909759000	-0.847304000
C	-1.890525000	-4.528506000	-1.050824000
C	-2.788285000	-4.650429000	0.005768000
C	-2.388298000	-5.314180000	1.180953000
C	-1.073146000	-5.702971000	1.373651000
C	0.443820000	-3.801904000	-2.840265000
C	-3.954461000	-3.724781000	-0.023739000
C	-4.679031000	-3.468035000	-1.203284000
C	-5.355537000	-2.273331000	-1.384325000
C	-5.313856000	-1.302182000	-0.382186000
C	-4.714803000	-1.633527000	0.850318000
C	-4.049405000	-2.838048000	1.044349000
C	-5.476314000	0.138704000	-0.376586000
C	-5.730702000	1.084313000	-1.371993000
C	-5.330692000	2.396390000	-1.182786000
C	-4.675411000	2.796954000	-0.002482000
C	-4.576232000	1.905032000	1.060977000
C	-4.965539000	0.585834000	0.859667000
C	-3.841656000	-0.419178000	2.845377000
N	-0.493795000	4.589539000	-1.637608000
N	4.661248000	0.508141000	1.643643000
N	0.521864000	-4.592731000	-1.636954000
N	-4.643085000	-0.504783000	1.649115000
H	-2.996541000	3.408983000	-1.915938000
H	-2.058158000	5.825914000	2.329091000
H	-4.194554000	4.648852000	2.006142000
H	2.201462000	3.967950000	-1.930763000
H	3.135015000	5.453566000	1.977443000
H	0.796109000	6.143420000	2.315729000
H	0.444122000	4.109949000	-3.425400000
H	-1.310804000	3.959094000	-3.437379000
H	4.664531000	4.196044000	-2.013032000
H	5.857468000	2.068731000	-2.336931000
H	3.465938000	3.003347000	1.923013000

H	6.178071000	-0.783180000	-2.323620000
H	5.476928000	-3.118327000	-1.983955000
H	4.028487000	-2.183021000	1.937865000
H	4.039948000	1.328340000	3.444904000
H	4.207871000	-0.425147000	3.440587000
H	3.026874000	-3.416764000	-1.916752000
H	2.084380000	-5.825209000	2.331768000
H	4.221911000	-4.650561000	2.007680000
H	-2.171422000	-3.962483000	-1.929926000
H	-3.107795000	-5.440793000	1.980728000
H	-0.770371000	-6.135544000	2.319796000
H	1.343261000	-3.958978000	-3.433354000
H	0.341125000	-2.734117000	-2.617782000
H	-4.629716000	-4.184382000	-2.014409000
H	-5.835487000	-2.063644000	-2.332763000
H	-3.440914000	-2.995890000	1.925541000
H	-6.153012000	0.779878000	-2.322210000
H	-5.439184000	3.111447000	-1.989159000
H	-4.012541000	2.183096000	1.942477000
H	-4.177479000	0.424524000	3.445950000
H	-2.779101000	-0.294332000	2.609798000
H	-3.974992000	-1.325147000	3.434071000
H	2.809176000	0.327369000	2.636665000
H	-0.410196000	-4.127626000	-3.431641000
H	-0.326528000	2.726420000	-2.611841000
H	-2.515931000	0.166944000	-0.273498000
H	-2.197256000	-0.500832000	-0.347116000

H₂O@TCC

C	2.604081000	-4.704095000	0.027239000
C	2.940928000	-3.875048000	1.092081000
C	3.941851000	-2.929455000	0.905640000
C	4.633956000	-2.808796000	-0.316772000
C	4.400370000	-3.758418000	-1.314279000
C	3.392969000	-4.691503000	-1.139545000
C	5.239719000	-1.489638000	-0.307824000
C	4.876315000	-0.900694000	0.922601000
C	4.919552000	0.475347000	1.119046000
C	5.301667000	1.287962000	0.054260000
C	5.816830000	0.698384000	-1.116051000
C	5.793253000	-0.674367000	-1.298687000
C	3.454269000	-1.480399000	2.880007000
C	4.736798000	2.667238000	0.060965000
C	4.699858000	3.462723000	1.221683000
C	3.731855000	4.439899000	1.390831000
C	2.765596000	4.628985000	0.400555000
C	2.905789000	3.929713000	-0.816441000
C	3.890521000	2.966982000	-1.003903000
C	1.427784000	5.189534000	0.387722000
C	0.606352000	5.759745000	1.362423000
C	-0.765091000	5.775424000	1.172779000
C	-1.346553000	5.232498000	0.011268000
C	-0.529234000	4.812504000	-1.033067000
C	0.845359000	4.784837000	-0.832107000
C	1.491486000	3.338816000	-2.773232000

C	-2.741787000	4.711572000	-0.013971000
C	-3.100249000	3.894104000	1.053753000
C	-4.099574000	2.948586000	0.858313000
C	-4.769172000	2.816882000	-0.375936000
C	-4.519763000	3.759842000	-1.374186000
C	-3.512000000	4.692332000	-1.191958000
C	-5.362403000	1.492827000	-0.373351000
C	-5.012483000	0.909877000	0.861623000
C	-5.043248000	-0.465150000	1.060114000
C	-5.410135000	-1.281318000	-0.005652000
C	-5.918511000	-0.698209000	-1.181714000
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C	-4.828668000	-3.452581000	1.176748000
C	-3.869428000	-4.434847000	1.360635000
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C	-3.020647000	-3.944298000	-0.843124000
C	-3.991207000	-2.970109000	-1.039930000
C	-1.562365000	-5.206044000	0.385968000
C	-0.749675000	-5.759487000	1.376816000
C	0.624556000	-5.771116000	1.202395000
C	1.216031000	-5.243250000	0.039682000
C	0.408531000	-4.846329000	-1.021503000
C	-0.967674000	-4.821841000	-0.833823000
C	-1.563556000	-3.419013000	-2.803303000
N	4.214438000	-1.829722000	1.703569000
N	1.793533000	4.139236000	-1.607698000
N	-4.379579000	1.851524000	1.655956000
N	-1.903619000	-4.181462000	-1.626074000
H	2.299296000	-3.837336000	1.962842000
H	4.941299000	-3.714366000	-2.251936000
H	3.144506000	-5.369965000	-1.946402000
H	4.463819000	0.920162000	1.994814000
H	6.146197000	1.340064000	-1.923901000
H	6.114249000	-1.098445000	-2.242674000
H	4.045328000	-0.814828000	3.507077000
H	3.242575000	-2.381318000	3.452332000
H	5.389446000	3.245926000	2.028470000
H	3.675451000	4.986664000	2.324458000
H	3.866977000	2.321371000	-1.873205000
H	1.026370000	6.112487000	2.296884000
H	-1.412375000	6.134481000	1.963603000
H	-0.971348000	4.333794000	-1.897001000
H	1.205323000	2.319416000	-2.494900000
H	2.367800000	3.299477000	-3.419136000
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H	-5.042918000	3.707544000	-2.321504000
H	-3.247008000	5.360924000	-2.001930000
H	-4.590581000	-0.904841000	1.939681000
H	-6.240559000	-1.344154000	-1.989453000
H	-6.215213000	1.094336000	-2.315373000
H	-3.493788000	2.432079000	3.439450000
H	-2.686932000	1.062963000	2.636305000
H	-5.525361000	-3.227230000	1.975038000
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H	-3.956542000	-2.324088000	-1.907622000
H	-1.177447000	-6.097370000	2.313231000
H	1.264129000	-6.112584000	2.007285000
H	0.854386000	-4.375143000	-1.888016000
H	-0.877948000	-3.997194000	-3.420976000
H	-1.096723000	-2.462941000	-2.543637000
H	-2.464810000	-3.233967000	-3.384632000
H	0.684811000	3.810034000	-3.330538000
H	-4.248461000	0.840416000	3.462762000
H	2.511707000	-0.989320000	2.615190000
O	2.302478000	0.047499000	-0.989827000
H	2.692692000	0.732918000	-0.435462000
H	3.006615000	-0.606250000	-1.077947000

H₂S@TCC

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C	-4.474680000	2.379644000	1.070919000
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C	-5.573464000	0.719542000	-0.352734000
C	-5.734075000	1.684000000	-1.349327000
C	-5.189137000	2.944364000	-1.169402000
C	-5.571241000	-0.731082000	-0.353544000
C	-5.005351000	-1.122322000	0.877330000
C	-4.468270000	-2.389556000	1.068734000
C	-4.473706000	-3.280865000	0.000257000
C	-5.180187000	-2.953985000	-1.172484000
C	-5.728677000	-1.694942000	-1.351221000
C	-4.005852000	-0.005242000	2.870951000
C	-3.396407000	-4.309428000	0.014722000
C	-3.064168000	-5.037878000	1.172509000
C	-1.790959000	-5.551287000	1.355741000
C	-0.817339000	-5.337024000	0.378150000
C	-1.205551000	-4.739137000	-0.838541000
C	-2.485564000	-4.236501000	-1.034664000
C	0.633237000	-5.326210000	0.387325000
C	1.598725000	-5.529075000	1.374503000
C	2.869382000	-5.003542000	1.203893000
C	3.207402000	-4.275778000	0.048304000
C	2.304913000	-4.209570000	-1.009807000
C	1.027580000	-4.723916000	-0.825976000
C	-0.079655000	-3.661223000	-2.791019000
C	4.289628000	-3.252648000	0.038940000
C	4.304403000	-2.371566000	1.115585000
C	4.857474000	-1.108205000	0.932784000
C	5.427858000	-0.717191000	-0.296059000
C	5.560927000	-1.672580000	-1.306456000
C	4.992067000	-2.923538000	-1.137476000
C	5.428764000	0.732325000	-0.296144000
C	4.856904000	1.123653000	0.931857000
C	4.299475000	2.385258000	1.112758000
C	4.282089000	3.264692000	0.035341000
C	4.986127000	2.936436000	-1.140562000
C	5.559293000	1.687168000	-1.307901000
C	3.801515000	0.008695000	2.892247000
C	3.197047000	4.284672000	0.044175000

C	2.858949000	5.013932000	1.198818000
C	1.587012000	5.535891000	1.370627000
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C	1.014998000	4.725446000	-0.827629000
C	2.293065000	4.213440000	-1.012073000
C	-0.830003000	5.335831000	0.377897000
C	-1.803161000	5.548200000	1.356369000
C	-3.075491000	5.031798000	1.174730000
C	-3.407501000	4.302607000	0.017379000
C	-2.497388000	4.231078000	-1.032733000
C	-1.218203000	4.736131000	-0.837909000
C	-0.093080000	3.658312000	-2.790179000
N	-4.809504000	-0.005717000	1.673039000
N	-0.085032000	-4.499058000	-1.615842000
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N	-0.098124000	4.497425000	-1.616061000
H	-3.877516000	2.599508000	1.946743000
H	-6.196781000	1.425126000	-2.294169000
H	-5.223201000	3.663585000	-1.978691000
H	-3.871037000	-2.608727000	1.944677000
H	-5.211987000	-3.672438000	-1.982549000
H	-6.191725000	-1.436333000	-2.295970000
H	-2.935072000	-0.004124000	2.640306000
H	-4.244489000	-0.886300000	3.464298000
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H	-1.533758000	-6.038681000	2.288527000
H	-2.711400000	-3.621607000	-1.896392000
H	1.337073000	-6.018104000	2.305164000
H	3.593948000	-5.080496000	2.005392000
H	2.535202000	-3.602493000	-1.876636000
H	-0.966028000	-3.872684000	-3.386450000
H	0.794809000	-3.895908000	-3.395893000
H	3.703276000	-2.587091000	1.989563000
H	6.020300000	-1.410920000	-2.252168000
H	5.007028000	-3.634111000	-1.954743000
H	3.696837000	2.599556000	1.985934000
H	4.999544000	3.646303000	-1.958481000
H	6.019434000	1.425706000	-2.253307000
H	4.015394000	-0.872543000	3.494407000
H	2.744587000	0.011628000	2.604663000
H	3.584584000	5.094472000	1.999012000
H	1.325387000	6.025767000	2.300852000
H	2.523295000	3.603736000	-1.876978000
H	-1.546104000	6.036397000	2.288782000
H	-3.806252000	5.113278000	1.970192000
H	-2.722661000	3.615390000	-1.894035000
H	-0.978436000	3.870687000	-3.386851000
H	-0.078991000	2.595074000	-2.527718000
H	0.782417000	3.890788000	-3.394377000
H	-0.063032000	-2.597712000	-2.529806000
H	4.019122000	0.887974000	3.495966000
H	-4.246181000	0.875070000	3.464699000
H	2.793461000	0.888518000	-0.872928000
H	2.656244000	-1.052177000	-0.736385000
S	1.826152000	-0.002664000	-0.582497000

CO@TCC

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C	1.407088000	-4.657003000	-0.984730000
C	0.056350000	-4.916484000	-0.789952000
C	-0.445074000	-5.379977000	0.444398000
C	0.465888000	-5.720547000	1.445613000
C	1.812207000	-5.451071000	1.262162000
C	-1.870359000	-5.108308000	0.427114000
C	-2.136916000	-4.495477000	-0.814963000
C	-3.289111000	-3.751249000	-1.035299000
C	-4.192392000	-3.597443000	0.012276000
C	-4.011806000	-4.339232000	1.195210000
C	-2.866360000	-5.088366000	1.405231000
C	-0.829353000	-3.746289000	-2.804997000
C	-5.031435000	-2.367761000	-0.031331000
C	-5.623438000	-1.905137000	-1.222153000
C	-5.893896000	-0.560500000	-1.414438000
C	-5.568739000	0.354934000	-0.411673000
C	-5.131761000	-0.141389000	0.834041000
C	-4.873213000	-1.491253000	1.037990000
C	-5.276284000	1.776181000	-0.403237000
C	-5.215628000	2.758295000	-1.393970000
C	-4.438862000	3.885438000	-1.187209000
C	-3.710399000	4.061635000	0.004710000
C	-3.907921000	3.180113000	1.063072000
C	-4.679552000	2.045159000	0.846059000
C	-3.986852000	0.749218000	2.862016000
C	-2.458060000	4.865915000	0.051806000
C	-1.572681000	4.666491000	-1.003393000
C	-0.221888000	4.913684000	-0.793140000
C	0.268126000	5.379739000	0.444910000
C	-0.652051000	5.733955000	1.433089000
C	-1.998252000	5.474874000	1.234837000
C	1.691041000	5.096256000	0.446790000
C	1.967753000	4.474451000	-0.788726000
C	3.120286000	3.726390000	-0.993972000
C	4.015535000	3.580732000	0.061906000
C	3.823460000	4.327181000	1.239940000
C	2.676728000	5.078521000	1.435122000
C	0.682940000	3.722654000	-2.790649000
C	4.867484000	2.360038000	0.026645000
C	5.461288000	1.898351000	-1.164734000
C	5.749732000	0.557357000	-1.350612000
C	5.440274000	-0.357305000	-0.341369000
C	4.998486000	0.138518000	0.902852000
C	4.725189000	1.488053000	1.101033000
C	5.134301000	-1.774749000	-0.340415000
C	5.060309000	-2.746830000	-1.341180000
C	4.268318000	-3.864406000	-1.145265000
C	3.534640000	-4.041638000	0.044315000
C	3.736650000	-3.168883000	1.108248000
C	4.525405000	-2.042432000	0.903134000
C	3.803128000	-0.741452000	2.901738000

N	-0.994394000	-4.515666000	-1.596557000
N	-4.735066000	0.912179000	1.639998000
N	0.835318000	4.497527000	-1.583534000
N	4.587041000	-0.913598000	1.702527000
H	1.744827000	-4.134042000	-1.870356000
H	0.117740000	-6.111805000	2.394100000
H	2.509837000	-5.631160000	2.071031000
H	-3.385129000	-3.134735000	-1.919804000
H	-4.743574000	-4.245075000	1.988441000
H	-2.710719000	-5.580577000	2.357801000
H	-1.742355000	-3.801393000	-3.395019000
H	-0.020594000	-4.172125000	-3.396639000
H	-5.783598000	-2.605268000	-2.033043000
H	-6.268239000	-0.216415000	-2.371183000
H	-4.360821000	-1.823370000	1.931757000
H	-5.695626000	2.602121000	-2.352707000
H	-4.311908000	4.603414000	-1.988343000
H	-3.303268000	3.271412000	1.956332000
H	-4.427057000	-0.054376000	3.450070000
H	-4.047616000	1.665557000	3.446443000
H	-1.904315000	4.139818000	-1.888970000
H	-0.311819000	6.127275000	2.383601000
H	-2.703864000	5.663174000	2.034919000
H	3.224447000	3.106065000	-1.875098000
H	4.548654000	4.238264000	2.039761000
H	2.513046000	5.576673000	2.383213000
H	-0.124427000	4.141616000	-3.388877000
H	0.463726000	2.672057000	-2.572502000
H	5.607433000	2.595845000	-1.980377000
H	6.120208000	0.212602000	-2.308557000
H	4.205254000	1.815679000	1.992089000
H	5.545507000	-2.589462000	-2.297044000
H	4.136295000	-4.575762000	-1.951399000
H	3.124184000	-3.255184000	1.996494000
H	2.762172000	-0.499332000	2.663130000
H	4.233580000	0.057858000	3.502645000
H	3.836904000	-1.657461000	3.488708000
H	-2.934701000	0.516986000	2.664713000
H	1.599665000	3.781646000	-3.374680000
H	-0.603085000	-2.696380000	-2.589113000
O	2.200905000	0.136269000	-1.364125000
C	2.246718000	-0.154011000	-0.279953000

CO₂@TCC

C	0.868436000	5.352868000	0.036426000
C	1.511585000	4.724114000	-
C	2.782555000	4.203595000	1.025811000
C	3.439929000	4.311164000	-
C	2.852362000	5.092730000	0.818132000
C	1.579791000	5.603112000	0.425048000
C	4.477149000	3.296019000	1.421550000
C	4.377499000	2.640877000	1.225100000
C	4.920094000	1.379795000	0.420520000
C	5.561659000	0.744491000	-
C	5.807932000	1.459030000	0.824457000
			-
			1.037262000

0	1	000
.	9	1.209714000
0	6	
2	7	

C	5.275784000	2.721685000	1.411329000
C	2.905528000	2.744746000	-2.836773000
C	5.561687000	-0.744302000	-0.021899000
C	5.808008000	-1.458813000	-1.209650000
C	5.275889000	-2.721473000	-1.411308000
C	4.477258000	-3.295852000	-0.420521000
C	4.377580000	-2.640744000	0.824470000
C	4.920128000	-1.379646000	1.037310000
C	3.440082000	-4.311039000	-0.425074000
C	2.852546000	-5.092600000	-1.421599000
C	1.579983000	-5.603012000	-1.225181000
C	0.868613000	-5.352823000	-0.036503000
C	1.511735000	-4.724080000	1.025757000
C	2.782689000	-4.203514000	0.818102000
C	2.905612000	-2.744710000	2.836781000
C	-0.619443000	-5.350749000	0.013563000
C	-1.267186000	-4.719771000	-1.044617000
C	-2.536221000	-4.196243000	-0.828178000
C	-3.182720000	-4.300887000	0.421198000
C	-2.591387000	-5.084079000	1.413778000
C	-1.323972000	-5.600585000	1.206722000
C	-4.221154000	-3.288808000	0.424280000
C	-4.141046000	-2.641798000	-0.826358000
C	-4.697869000	-1.386779000	-1.043107000
C	-5.322631000	-0.744409000	0.024168000
C	-5.546780000	-1.452124000	1.220254000
C	-5.008793000	-2.711784000	1.421797000
C	-2.705656000	-2.753270000	-2.864320000
C	-5.322645000	0.744269000	-0.024142000
C	-5.546830000	1.451962000	-1.220230000
C	-5.008872000	2.711630000	-1.421800000
C	-4.221257000	3.288698000	-0.424293000
C	-4.141124000	2.641712000	0.826354000
C	-4.697896000	1.386671000	1.043122000
C	-3.182879000	4.300834000	-0.421219000
C	-2.591583000	5.084035000	-1.413813000
C	-1.324173000	5.600564000	-1.206789000
C	-0.619621000	5.350761000	-0.013634000
C	-1.267338000	4.719786000	1.044565000
C	-2.536359000	4.196218000	0.828149000
C	-2.705727000	2.753252000	2.864300000
N	3.449901000	3.292864000	-1.618997000
N	3.450002000	-3.292781000	1.618992000
N	-3.215212000	-3.290088000	-1.625746000
N	-3.215326000	3.290061000	1.625738000
H	0.951602000	4.469455000	-1.916371000
H	3.345798000	5.227674000	2.376623000
H	1.083999000	6.130797000	2.030957000
H	4.669881000	0.816523000	-1.927020000
H	6.346040000	0.970052000	2.012821000
H	5.406482000	3.215459000	2.366827000
H	3.708680000	2.301777000	-3.423218000
H	2.461511000	3.545578000	-3.425790000
H	6.346116000	-0.969803000	-2.012737000
H	5.406620000	-3.215224000	-2.366813000
H	4.669876000	-0.816404000	1.927076000

H	3.345992000	-5.227496000	-2.376674000
H	1.084212000	-6.130684000	-2.031060000
H	0.951731000	-4.469469000	1.916317000
H	3.708754000	-2.301752000	3.423251000
H	2.461596000	-3.545566000	3.425765000
H	-0.712560000	-4.469197000	-1.939772000
H	-3.078633000	-5.216458000	2.372301000
H	-0.823879000	-6.130871000	2.008109000
H	-4.465487000	-0.832286000	-1.943519000
H	-6.072821000	-0.959625000	2.029044000
H	-5.122286000	-3.198633000	2.382907000
H	-2.229593000	-3.550543000	-3.432325000
H	-1.982436000	-1.948864000	-2.693465000
H	-6.072865000	0.959437000	-2.029006000
H	-5.122393000	3.198464000	-2.382914000
H	-4.465487000	0.832200000	1.943540000
H	-3.078843000	5.216379000	-2.372334000
H	-0.824106000	6.130850000	-2.008191000
H	-0.712691000	4.469247000	1.939717000
H	-2.229661000	3.550533000	3.432291000
H	-1.982498000	1.948858000	2.693422000
H	-3.533416000	2.365604000	3.456416000
H	2.144690000	-1.983210000	2.634307000
H	-3.533367000	-2.365632000	-3.456413000
H	2.144613000	1.983245000	-2.634281000
O	-2.078018000	-0.456919000	1.061773000
C	-2.096442000	-0.000235000	0.000107000
O	-2.077957000	0.456450000	-1.061555000

CS₂@TCC

C	-5.258018000	-0.746520000	-0.004405000
C	-4.621947000	-1.361194000	1.069678000
C	-4.096329000	-2.634366000	0.886826000
C	-4.217430000	-3.324017000	-0.336747000
C	-5.007099000	-2.763185000	-1.342329000
C	-5.515169000	-1.486123000	-1.174358000
C	-3.175453000	-4.333345000	-0.334307000
C	-2.492809000	-4.188217000	0.891327000
C	-1.214809000	-4.697643000	1.086159000
C	-0.588137000	-5.346030000	0.026108000
C	-1.316566000	-5.619627000	-1.146972000
C	-2.597316000	-5.124381000	-1.329030000
C	-2.565114000	-2.647829000	2.850226000
C	0.900341000	-5.345659000	0.053563000
C	1.626842000	-5.605685000	1.230459000
C	2.902414000	-5.097798000	1.413515000
C	3.475898000	-4.308324000	0.415494000
C	2.801341000	-4.188281000	-0.817323000
C	1.527595000	-4.707314000	-1.012154000
C	4.514258000	-3.294483000	0.406193000
C	5.324749000	-2.729747000	1.392737000
C	5.855307000	-1.465536000	1.196176000
C	5.596943000	-0.741921000	0.016883000
C	4.941621000	-1.366660000	-1.040141000
C	4.398699000	-2.628095000	-0.831225000

C	2.891467000	-2.703768000	-2.817570000
C	5.596166000	0.747167000	-0.016791000
C	4.940185000	1.371236000	1.040214000
C	4.396073000	2.632147000	0.831315000
C	4.511050000	3.298671000	-0.406069000
C	5.322121000	2.734760000	-1.392608000
C	5.853874000	1.471042000	-1.196065000
C	3.471818000	4.311619000	-0.415337000
C	2.797338000	4.190932000	0.817457000
C	1.523126000	4.708810000	1.012262000
C	0.895317000	5.346551000	-0.053491000
C	1.621604000	5.607258000	-1.230370000
C	2.897651000	5.100556000	-1.413394000
C	2.888424000	2.705936000	2.817309000
C	-0.593154000	5.345514000	-0.026090000
C	-1.321873000	5.618548000	1.146943000
C	-2.602190000	5.122178000	1.329007000
C	-3.179608000	4.330529000	0.334355000
C	-2.496764000	4.185881000	-0.891245000
C	-1.219211000	4.696432000	-1.086100000
C	-4.220661000	3.320246000	0.336871000
C	-5.009729000	2.758685000	1.342525000
C	-5.516602000	1.481134000	1.174648000
C	-5.258751000	0.741673000	0.004753000
C	-4.623252000	1.356870000	-1.069377000
C	-4.098922000	2.630612000	-0.886647000
C	-2.567959000	2.645403000	-2.850218000
N	-3.148784000	-3.258770000	1.680588000
N	3.458644000	-3.270933000	-1.618943000
N	3.455468000	3.274133000	1.619084000
N	-3.151802000	3.255675000	-1.680355000
H	-4.354642000	-0.775152000	1.940262000
H	-5.144264000	-3.278412000	-2.285476000
H	-6.046314000	-1.008703000	-1.988897000
H	-0.638268000	-4.422212000	1.959912000
H	-0.829672000	-6.156788000	-1.951930000
H	-3.107191000	-5.280428000	-2.272177000
H	-2.070631000	-3.411356000	3.447894000
H	-3.352403000	-2.203402000	3.456783000
H	1.140543000	-6.138473000	2.038704000
H	3.408877000	-5.240305000	2.360588000
H	0.954371000	-4.446782000	-1.892855000
H	5.465315000	-3.231766000	2.342485000
H	6.401521000	-0.982749000	1.997544000
H	4.682223000	-0.794492000	-1.921628000
H	2.434654000	-3.495090000	-3.409646000
H	3.683561000	-2.253255000	-3.413151000
H	4.681347000	0.798793000	1.921687000
H	5.462246000	3.236961000	-2.342323000
H	6.400586000	0.988789000	-1.997414000
H	0.950063000	4.447692000	1.892898000
H	1.134827000	6.139617000	-2.038609000
H	3.404031000	5.243541000	-2.360437000
H	3.680817000	2.256447000	3.413265000
H	2.134437000	1.945282000	2.586538000
H	-0.835489000	6.156175000	1.951908000

H	-3.112220000	5.277832000	2.272136000
H	-0.642441000	4.421454000	-1.959843000
H	-5.147362000	3.273837000	2.285647000
H	-6.047279000	1.003281000	1.989236000
H	-4.355314000	0.771020000	-1.939888000
H	-3.355087000	2.200849000	-3.456901000
H	-1.840554000	1.870953000	-2.580019000
H	-2.073691000	3.409281000	-3.447616000
H	2.136286000	-1.944122000	-2.587402000
H	2.430170000	3.496509000	3.409265000
H	-1.837936000	-1.873241000	2.579789000
C	-1.536393000	-0.000770000	-0.000523000
S	-1.545853000	1.274591000	0.889545000
S	-1.545117000	-	-0.890522000
		1.276189000	

N₂@TCC

C	-3.125482000	4.503861000	0.018500000
C	-2.217808000	4.422651000	-1.033734000
C	-0.915779000	4.858180000	-0.821930000
C	-0.500313000	5.394208000	0.414946000
C	-1.465146000	5.629329000	1.395903000
C	-2.761292000	5.184834000	1.195570000
C	0.947138000	5.300254000	0.428382000
C	1.313461000	4.715055000	-0.801730000
C	2.556664000	4.124503000	-0.993195000
C	3.452016000	4.098074000	0.072514000
C	3.151512000	4.812627000	1.247224000
C	1.915909000	5.412189000	1.426971000
C	0.152468000	3.789850000	-2.807227000
C	4.460612000	3.003174000	0.044606000
C	5.131146000	2.636753000	-1.138538000
C	5.612135000	1.351758000	-1.323655000
C	5.419983000	0.397750000	-0.322541000
C	4.887580000	0.818589000	0.913508000
C	4.423822000	2.113341000	1.113356000
C	5.324799000	-1.049087000	-0.329889000
C	5.414718000	-2.014569000	-1.334328000
C	4.792377000	-3.238920000	-1.158256000
C	4.076733000	-3.530707000	0.018647000
C	4.127686000	-2.643224000	1.089173000
C	4.739767000	-1.409672000	0.901592000
C	3.798768000	-0.231828000	2.889394000
C	2.954574000	-4.508727000	0.040945000
C	2.056287000	-4.425723000	-1.018892000
C	0.755206000	-4.871090000	-0.821875000
C	0.330385000	-5.414943000	0.408554000
C	1.286532000	-5.646631000	1.398807000
C	2.582171000	-5.194863000	1.212340000
C	-1.117887000	-5.332199000	0.406746000
C	-1.475325000	-4.745919000	-0.825115000
C	-2.719215000	-4.160476000	-1.026646000
C	-3.623391000	-4.137037000	0.031384000
C	-3.331210000	-4.853443000	1.207315000
C	-2.095521000	-5.449808000	1.396400000
C	-0.298242000	-3.804987000	-2.814814000

C	-4.625504000	-3.035550000	-0.001326000
C	-5.297591000	-2.670754000	-1.183475000
C	-5.757368000	-1.379381000	-1.378369000
C	-5.547661000	-0.420101000	-0.385971000
C	-5.024910000	-0.840267000	0.854911000
C	-4.573513000	-2.138021000	1.060984000
C	-5.462468000	1.027992000	-0.389056000
C	-5.558469000	1.999956000	-1.386344000
C	-4.950868000	3.230166000	-1.198313000
C	-4.244917000	3.521997000	-0.015915000
C	-4.296859000	2.628403000	1.050033000
C	-4.892978000	1.389293000	0.849580000
C	-3.991779000	0.220466000	2.861464000
N	0.193188000	4.585249000	-1.604715000
N	4.617728000	-0.286239000	1.702765000
N	-0.347055000	-4.604103000	-1.615381000
N	-4.771552000	0.265163000	1.649085000
H	-2.468252000	3.843703000	-1.913520000
H	-1.186219000	6.073275000	2.344152000
H	-3.489788000	5.279549000	1.991636000
H	2.755090000	3.526647000	-1.873660000
H	3.872698000	4.818687000	2.055511000
H	1.679348000	5.887317000	2.371498000
H	1.058261000	3.964599000	-3.385201000
H	-0.698361000	4.095058000	-3.414128000
H	5.190481000	3.352678000	-1.949245000
H	6.044073000	1.068335000	-2.276050000
H	3.847261000	2.358694000	1.996243000
H	5.886636000	-1.780413000	-2.281036000
H	4.776937000	-3.954801000	-1.971166000
H	3.521718000	-2.830575000	1.966149000
H	4.121635000	0.599403000	3.514442000
H	3.929627000	-1.149452000	3.459593000
H	2.312032000	-3.841172000	-1.893794000
H	1.000911000	-6.095442000	2.342766000
H	3.303863000	-5.289086000	2.014635000
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H	-4.058355000	-4.860978000	2.010301000
H	-1.865323000	-5.925080000	2.342397000
H	0.556083000	-4.108385000	-3.417880000
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H	-4.937597000	3.950678000	-2.007176000
H	-3.703676000	2.818376000	1.935255000
H	-4.174510000	1.124383000	3.439753000
H	-2.919948000	0.137647000	2.650938000
H	-4.304793000	-0.632212000	3.461960000
H	2.739515000	-0.107614000	2.639330000
H	-1.200518000	-3.977325000	-3.398741000
H	0.070309000	2.720875000	-2.583900000
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N	2.179663000	0.162506000	-0.221800000

NO@TCC

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C	1.212190000	-4.745272000	-0.976969000
C	-0.148711000	-4.949755000	-0.788250000
C	-0.674599000	-5.388089000	0.445080000
C	0.217296000	-5.761069000	1.452186000
C	1.574191000	-5.545797000	1.274909000
C	-2.087248000	-5.056639000	0.420781000
C	-2.321890000	-4.436211000	-0.824036000
C	-3.437402000	-3.639765000	-1.050574000
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C	-4.195035000	-4.190048000	1.177807000
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C	-0.977773000	-3.751211000	-2.811689000
C	-5.118980000	-2.176053000	-0.052700000
C	-5.685792000	-1.685370000	-1.244481000
C	-5.902298000	-0.330236000	-1.432111000
C	-5.546280000	0.567864000	-0.424073000
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C	-4.929335000	-1.310273000	1.020244000
C	-5.201351000	1.977331000	-0.407422000
C	-5.101602000	2.962768000	-1.392027000
C	-4.284042000	4.058901000	-1.176283000
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C	-3.784529000	3.320445000	1.070430000
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C	-3.962378000	0.887505000	2.857183000
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C	-1.395392000	4.740234000	-0.988350000
C	-0.036120000	4.935559000	-0.778438000
C	0.473063000	5.366983000	0.464371000
C	-0.431886000	5.743010000	1.458759000
C	-1.786971000	5.535959000	1.260417000
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C	2.134138000	4.410335000	-0.782238000
C	3.251365000	3.613116000	-0.997463000
C	4.134456000	3.408723000	0.058495000
C	3.976595000	4.150011000	1.245292000
C	2.867317000	4.952480000	1.449390000
C	0.819963000	3.731773000	-2.789528000
C	4.924867000	2.147718000	0.017094000
C	5.493009000	1.657125000	-1.173639000
C	5.728993000	0.303384000	-1.354591000
C	5.389634000	-0.594962000	-0.342005000
C	4.964164000	-0.077317000	0.899526000
C	4.743987000	1.282799000	1.092456000
C	5.033525000	-2.001223000	-0.334048000
C	4.933033000	-2.978482000	-1.326830000
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C	3.355551000	-4.207698000	0.059540000
C	3.582813000	-3.334593000	1.118510000
C	4.411515000	-2.239044000	0.908784000
C	3.729320000	-0.901067000	2.897053000

N	-1.178442000	-4.508306000	-1.601021000
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H	-0.724843000	-2.706715000	-2.599178000
H	-1.884963000	-3.784199000	-3.412447000
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H	-5.584710000	2.830296000	-2.352774000
H	-4.129726000	4.777080000	-1.972392000
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H	2.964712000	-3.394582000	2.005071000
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H	2.696895000	-0.628207000	2.653616000
H	4.181227000	-0.109750000	3.492604000
H	-2.916041000	0.627717000	2.663187000
H	1.732833000	3.771620000	-3.381333000
H	-0.174352000	-4.203495000	-3.390658000
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O	2.457115000	0.352170000	-1.384236000

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C	2.715164000	5.158490000	0.811710000
C	1.425732000	5.627638000	0.428475000
C	4.392255000	3.418280000	1.429952000
C	4.306777000	2.761392000	1.241162000
C	4.887579000	1.517979000	0.416863000
C	5.554677000	0.902925000	-
C	5.786377000	1.624974000	0.828112000
			-
			1.044731000

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C	5.215104000	2.869706000	1.402524000
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C	4.585203000	-3.167225000	-0.420390000
C	4.472483000	-2.512712000	0.823798000
C	4.980492000	-1.236605000	1.031815000
C	3.575880000	-4.210082000	-0.419169000
C	3.006951000	-5.009222000	-1.412474000
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C	1.033412000	-5.316697000	-0.022147000
C	1.662486000	-4.669924000	1.037554000
C	2.919340000	-4.117268000	0.825555000
C	3.012441000	-2.652039000	2.841846000
C	-0.454223000	-5.352813000	0.027367000
C	-1.114715000	-4.735283000	-1.030864000
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C	-3.051866000	-4.385520000	0.423670000
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C	-4.324946000	3.164953000	-0.391889000
C	-4.218971000	2.507458000	0.850778000
C	-4.738751000	1.234856000	1.056891000
C	-3.309399000	4.200683000	-0.387181000
C	-2.745928000	5.008960000	-1.375727000
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N	3.354844000	3.384618000	-1.617106000
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H	3.208853000	5.306672000	2.382919000
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H	-4.482327000	0.675521000	1.947932000
H	-3.244575000	5.140354000	-2.328469000
H	-1.009926000	6.106808000	-1.972263000
H	-0.822883000	4.403130000	1.954159000
H	-2.261326000	3.389258000	3.431526000
H	-2.012576000	1.815920000	2.634888000
H	-3.545056000	2.183426000	3.461505000
H	2.585001000	-3.462149000	3.430397000
H	-3.409940000	-2.411412000	-3.436035000
H	2.354806000	3.610867000	-3.420953000
O	-2.080651000	-0.705143000	0.704082000
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N	-2.132481000	0.267168000	0.033624000

F₂@TCC

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C	-3.157686000	-4.495723000	0.429680000
C	-2.529857000	-5.235497000	1.433552000
C	-1.227342000	-5.667997000	1.247630000
C	-4.254662000	-3.545870000	0.414729000
C	-4.185615000	-2.888581000	-0.831040000
C	-4.800345000	-1.661987000	-1.050567000
C	-5.487633000	-1.065075000	0.002087000
C	-5.702249000	-1.792485000	1.188066000
C	-5.095778000	-3.019919000	1.397380000
C	-2.700354000	-2.912230000	-2.835801000
C	-5.576199000	0.421107000	-0.040534000
C	-5.854187000	1.123352000	-1.228750000
C	-5.399184000	2.417177000	-1.421038000
C	-4.646611000	3.036105000	-0.421015000
C	-4.517328000	2.383158000	0.822342000
C	-4.983961000	1.090758000	1.026231000
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C	-3.129403000	4.934628000	-1.401854000
C	-1.891025000	5.519327000	-1.195049000
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C	-1.780974000	4.632459000	1.050866000
C	-3.018232000	4.038553000	0.833547000

C	-3.074302000	2.567633000	2.848368000
C	0.315322000	5.383982000	0.044018000
C	0.991461000	4.787940000	-1.016630000
C	2.290496000	4.341051000	-0.809973000
C	2.942405000	4.492188000	0.431965000
C	2.311650000	5.240194000	1.427751000
C	1.012111000	5.676550000	1.231818000
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C	3.987058000	2.887807000	-0.818125000
C	4.613655000	1.666641000	-1.034310000
C	5.290309000	1.071285000	0.025843000
C	5.488293000	1.798790000	1.215082000
C	4.876004000	3.023908000	1.418355000
C	2.507952000	2.881085000	-2.823578000
C	5.379684000	-0.414373000	-0.013331000
C	5.649964000	-1.117001000	-1.203395000
C	5.191614000	-2.409623000	-1.394074000
C	4.440492000	-3.026133000	-0.391146000
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C	4.791588000	-1.083094000	1.056246000
C	3.461688000	-4.096643000	-0.383958000
C	2.924175000	-4.925443000	-1.370438000
C	1.686839000	-5.512490000	-1.165559000
C	0.960296000	-5.289504000	0.019292000
C	1.561847000	-4.607519000	1.072814000
C	2.800023000	-4.013886000	0.858965000
C	2.851053000	-2.524048000	2.861940000
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N	-3.636520000	3.086546000	1.626187000
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H	-3.526683000	-2.524021000	-3.428917000
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H	4.974072000	3.523981000	2.374543000
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H	1.225249000	-6.082088000	-1.963025000
H	0.986362000	-4.377608000	1.960325000
H	2.404663000	-3.330855000	3.440414000
H	2.088045000	-1.767668000	2.647867000
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H	3.342063000	2.526735000	-3.427214000
H	-1.989973000	-2.103219000	-2.633901000
F	2.278907000	-0.522316000	-0.748458000
F	2.061284000	0.387531000	0.253860000

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C	1.518955000	-5.487241000	1.448750000
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C	-0.892839000	-5.306596000	0.438742000
C	-1.274389000	-4.731561000	-0.790921000
C	-2.554232000	-4.236463000	-1.005251000
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C	-5.108560000	-1.116205000	0.869486000
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C	-2.553708000	4.236886000	-1.005048000
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C	-0.891989000	5.306721000	0.438812000
C	-1.872618000	5.511244000	1.411280000
C	-3.147023000	5.008580000	1.208646000
C	0.558165000	5.293418000	0.456605000
C	0.959698000	4.712905000	-0.765342000
C	2.242087000	4.210919000	-0.954579000
C	3.144400000	4.269399000	0.106929000
C	2.796010000	4.976071000	1.271963000
C	1.519956000	5.487175000	1.448506000
C	-0.137896000	3.704583000	-2.765868000
C	4.241611000	3.263588000	0.080245000

C	4.913247000	2.936103000	-1.113464000
C	5.465969000	1.682033000	-1.302905000
C	5.347836000	0.724047000	-0.294188000
C	4.821476000	1.117145000	0.952724000
C	4.285341000	2.383279000	1.156209000
C	5.347728000	-0.724853000	-0.294114000
C	5.465775000	-1.682961000	-1.302710000
C	4.912883000	-2.936931000	-1.113150000
C	4.241137000	-3.264189000	0.080564000
C	4.284964000	-2.383778000	1.156457000
C	4.821307000	-1.117737000	0.952841000
C	3.847963000	-0.000114000	2.956995000
N	-0.148807000	-4.504055000	-1.564854000
N	-4.929577000	0.000263000	1.669368000
N	-0.148286000	4.504054000	-1.564861000
N	4.642543000	-0.000238000	1.752359000
H	2.486353000	-3.634484000	-1.837858000
H	1.251636000	-5.960187000	2.386164000
H	3.517662000	-5.049720000	2.075901000
H	-2.774534000	-3.635646000	-1.878262000
H	-3.886149000	-5.084506000	1.997382000
H	-1.622323000	-5.983101000	2.353317000
H	-0.134577000	-2.633761000	-2.537782000
H	-1.015662000	-3.943689000	-3.364252000
H	-5.254090000	-3.666192000	-1.993722000
H	-6.228462000	-1.431451000	-2.327586000
H	-3.992906000	-2.599341000	1.959222000
H	-6.228419000	1.432641000	-2.327361000
H	-5.253738000	3.667210000	-1.993279000
H	-3.992368000	2.599676000	1.959428000
H	-4.402625000	-0.880507000	3.472208000
H	-4.402454000	0.880763000	3.472288000
H	-2.774200000	3.636160000	-1.878072000
H	-1.621163000	5.983192000	2.353525000
H	-3.885133000	5.084843000	1.997835000
H	2.486700000	3.634015000	-1.838060000
H	3.518701000	5.049536000	2.075402000
H	1.252819000	5.960250000	2.385903000
H	-0.134384000	2.633704000	-2.537689000
H	0.746280000	3.948434000	-3.352775000
H	4.910157000	3.648835000	-1.929160000
H	5.896959000	1.419596000	-2.261636000
H	3.706767000	2.597729000	2.045677000
H	5.896855000	-1.420700000	-2.261443000
H	4.909734000	-3.649762000	-1.928761000
H	3.706302000	-2.598042000	2.045923000
H	4.090949000	-0.880662000	3.549143000
H	2.775627000	-0.000038000	2.731372000
H	4.091093000	0.880446000	3.549060000
H	-3.075699000	0.000035000	2.675379000
H	-1.015427000	3.943689000	-3.364123000
H	0.746041000	-3.948629000	-3.352688000
Cl	1.741342000	-1.018156000	-0.656666000
Cl	1.741479000	1.017847000	-0.656716000

Br₂@TCC

C	-3.574305000	4.301162000	0.058696000
C	-2.653545000	4.258610000	-0.983646000
C	-1.373599000	4.748569000	-0.756830000
C	-0.993155000	5.297086000	0.484862000
C	-1.975889000	5.487105000	1.458296000
C	-3.250586000	4.992415000	1.242039000
C	0.456265000	5.280585000	0.505235000
C	0.859930000	4.724975000	-0.728337000
C	2.144738000	4.228755000	-0.924423000
C	3.047545000	4.270703000	0.139343000
C	2.695175000	4.956026000	1.315735000
C	1.417007000	5.458775000	1.500740000
C	-0.241975000	3.790374000	-2.769147000
C	4.147276000	3.268124000	0.099713000
C	4.802419000	2.940078000	-1.103235000
C	5.349314000	1.684957000	-1.302033000
C	5.242033000	0.724982000	-0.293580000
C	4.733104000	1.118008000	0.960629000
C	4.204555000	2.385986000	1.173524000
C	5.242191000	-0.723740000	-0.293675000
C	5.349609000	-1.683556000	-1.302271000
C	4.803002000	-2.938829000	-1.103614000
C	4.148037000	-3.267196000	0.099341000
C	4.205166000	-2.385177000	1.173252000
C	4.733383000	-1.117044000	0.960498000
C	3.784812000	0.000246000	2.977552000
C	3.048576000	-4.270068000	0.138980000
C	2.145622000	-4.228226000	-0.924662000
C	0.860959000	-4.724774000	-0.728456000
C	0.457568000	-5.280503000	0.505150000
C	1.418485000	-5.458597000	1.500498000
C	2.696530000	-4.955597000	1.315341000
C	-0.991853000	-5.297286000	0.484967000
C	-1.372571000	-4.748899000	-0.756703000
C	-2.652658000	-4.259260000	-0.983398000
C	-3.573275000	-4.301915000	0.059067000
C	-3.249242000	-4.992965000	1.242443000
C	-1.974420000	-5.487404000	1.458558000
C	-0.241401000	-3.790420000	-2.769135000
C	-4.651569000	-3.275879000	0.012020000
C	-5.326986000	-2.950946000	-1.179663000
C	-5.869511000	-1.691941000	-1.375748000
C	-5.739565000	-0.726053000	-0.375820000
C	-5.209436000	-1.116720000	0.870977000
C	-4.676776000	-2.382713000	1.078554000
C	-5.739726000	0.724714000	-0.375914000
C	-5.869807000	1.690437000	-1.375991000
C	-5.327565000	2.949590000	-1.180050000
C	-4.652342000	3.274856000	0.011654000
C	-4.677422000	2.381823000	1.078301000
C	-5.209733000	1.115669000	0.870852000
C	-4.259093000	-0.000288000	2.887722000
N	-0.247096000	4.535268000	-1.533296000
N	4.562314000	0.000413000	1.761462000
N	-0.246205000	-4.535331000	-1.533293000

N	-5.035584000	-0.000457000	1.671941000
H	-2.870683000	3.672756000	-1.867595000
H	-1.726050000	5.941213000	2.409688000
H	-3.991054000	5.056891000	2.030054000
H	2.391829000	3.670665000	-1.818925000
H	3.416642000	5.018424000	2.121163000
H	1.147767000	5.914144000	2.446272000
H	-0.272720000	2.710544000	-2.591974000
H	0.656910000	4.035256000	-3.332679000
H	4.791582000	3.653844000	-1.917986000
H	5.767657000	1.423708000	-2.266644000
H	3.636127000	2.597725000	2.070114000
H	5.767827000	-1.422076000	-2.266875000
H	4.792273000	-3.652477000	-1.918469000
H	3.636852000	-2.597172000	2.069853000
H	2.709407000	0.000131000	2.767285000
H	4.036448000	0.880692000	3.566291000
H	2.392483000	-3.670042000	-1.819168000
H	1.149471000	-5.914097000	2.446031000
H	3.418128000	-5.017926000	2.120654000
H	-2.870041000	-3.673535000	-1.867372000
H	-3.989580000	-5.057504000	2.030576000
H	-1.724356000	-5.941377000	2.409959000
H	-0.272401000	-2.710600000	-2.591947000
H	-1.103845000	-4.081835000	-3.366694000
H	-5.338171000	-3.670614000	-1.989228000
H	-6.306022000	-1.435213000	-2.333574000
H	-4.102916000	-2.597989000	1.970641000
H	-6.306181000	1.433471000	-2.333818000
H	-5.338836000	3.669130000	-1.989728000
H	-4.103684000	2.597359000	1.970401000
H	-3.183379000	-0.000169000	2.680641000
H	-4.511437000	-0.880818000	3.476036000
H	-4.511653000	0.880251000	3.475929000
H	4.036658000	-0.880212000	3.566182000
H	0.657485000	-4.035072000	-3.332765000
H	-1.104428000	4.081581000	-3.366793000
Br	1.371258000	1.163372000	-0.424149000
Br	1.371488000	-1.163086000	-0.424208000

HF@TCC

C	-1.386779000	5.234868000	0.086403000
C	-0.575456000	4.875991000	-0.985657000
C	0.802300000	4.890778000	-0.808235000
C	1.393855000	5.277832000	0.412282000
C	0.572277000	5.796119000	1.414873000
C	-0.802893000	5.768269000	1.250538000
C	2.743773000	4.746586000	0.391161000
C	2.878815000	4.070558000	-0.839148000
C	3.871417000	3.121772000	-1.051127000
C	4.738865000	2.822081000	-0.005211000
C	4.709919000	3.604793000	1.164907000
C	3.727122000	4.559977000	1.364823000
C	1.433149000	3.536473000	-2.804066000
C	5.338302000	1.458899000	-0.035107000

C	5.850631000	0.891368000	-1.216965000
C	5.877931000	-0.481084000	-1.400373000
C	5.382397000	-1.316876000	-0.398042000
C	5.024313000	-0.743607000	0.839540000
C	5.009454000	0.631984000	1.034959000
C	4.845025000	-2.664479000	-0.388384000
C	4.626380000	-3.625011000	-1.377429000
C	3.663247000	-4.599889000	-1.176822000
C	2.904912000	-4.643090000	0.008570000
C	3.239809000	-3.803783000	1.066928000
C	4.196223000	-2.818392000	0.854171000
C	3.719812000	-1.413221000	2.858716000
C	1.532465000	-5.220690000	0.047633000
C	0.696105000	-4.851636000	-1.001013000
C	-0.677779000	-4.869034000	-0.794171000
C	-1.241261000	-5.270803000	0.435616000
C	-0.395722000	-5.794738000	1.415748000
C	0.975026000	-5.763978000	1.220777000
C	-2.595176000	-4.749532000	0.447219000
C	-2.760546000	-4.070120000	-0.777285000
C	-3.761365000	-3.125852000	-0.967973000
C	-4.605134000	-2.832861000	0.097818000
C	-4.548030000	-3.615742000	1.266706000
C	-3.558687000	-4.569217000	1.442503000
C	-1.373190000	-3.482383000	-2.756744000
C	-5.196241000	-1.465965000	0.086195000
C	-5.744187000	-0.893520000	-1.078632000
C	-5.771015000	0.482524000	-1.260531000
C	-5.238167000	1.317666000	-0.272365000
C	-4.840560000	0.737020000	0.953403000
C	-4.828167000	-0.639635000	1.144127000
C	-4.698748000	2.665076000	-0.274141000
C	-4.511725000	3.631957000	-1.264589000
C	-3.547167000	4.608212000	-1.084323000
C	-2.754690000	4.646291000	0.079486000
C	-3.054631000	3.798552000	1.140676000
C	-4.012757000	2.811046000	0.948118000
C	-3.471849000	1.395999000	2.931777000
N	1.751626000	4.286818000	-1.613370000
N	4.439059000	-1.707071000	1.643922000
N	-1.648321000	-4.265568000	-1.574335000
N	-4.227309000	1.693612000	1.738604000
H	-1.013416000	4.400337000	-1.853743000
H	0.996803000	6.136213000	2.351963000
H	-1.446090000	6.080932000	2.064199000
H	3.846606000	2.483722000	-1.925194000
H	5.418022000	3.390546000	1.956183000
H	3.674495000	5.092204000	2.307075000
H	1.025006000	2.549113000	-2.563422000
H	2.332649000	3.417790000	-3.405611000
H	6.142379000	1.546188000	-2.029034000
H	6.197218000	-0.892371000	-2.350573000
H	4.553593000	1.058015000	1.919486000
H	5.136586000	-3.557361000	-2.330850000
H	3.420537000	-5.286406000	-1.978756000
H	2.620869000	-3.789410000	1.955103000

H	2.714048000	-1.031357000	2.652475000
H	4.273057000	-0.672632000	3.433759000
H	1.115991000	-4.371719000	-1.875371000
H	-0.798958000	-6.144866000	2.358561000
H	1.637142000	-6.084701000	2.015860000
H	-3.743126000	-2.480943000	-1.836897000
H	-5.237756000	-3.404020000	2.074876000
H	-3.484358000	-5.102630000	2.382590000
H	-1.081001000	-2.459147000	-2.501277000
H	-2.263905000	-3.450756000	-3.382644000
H	-6.063411000	-1.544916000	-1.882705000
H	-6.122190000	0.896189000	-2.198497000
H	-4.346053000	-1.070331000	2.012187000
H	-5.049901000	3.569841000	-2.202793000
H	-3.330865000	5.302197000	-1.887235000
H	-2.410787000	3.780861000	2.010651000
H	-3.384866000	2.297444000	3.536023000
H	-2.470917000	1.022533000	2.692113000
H	-4.004395000	0.648361000	3.516767000
H	3.643551000	-2.317824000	3.459962000
H	-0.578665000	-3.960768000	-3.325762000
H	0.704644000	4.090492000	-3.393839000
H	-3.532650000	0.140488000	-1.477625000
F	-2.678319000	-0.075686000	-1.776198000

HCl@TCC

C	3.700323000	-4.077001000	0.013582000
C	3.898395000	-3.196022000	1.072192000
C	4.679792000	-2.067184000	0.857799000
C	5.285888000	-1.805134000	-0.388507000
C	5.224116000	-2.788277000	-1.377993000
C	4.437077000	-3.908770000	-1.174213000
C	5.586424000	-0.385653000	-0.399167000
C	5.144916000	0.116696000	0.842543000
C	4.891553000	1.468457000	1.040424000
C	5.058110000	2.339950000	-0.031709000
C	5.653326000	1.870824000	-1.218165000
C	5.919941000	0.524484000	-1.403876000
C	3.979402000	-0.761041000	2.863960000
C	4.222104000	3.572058000	0.003213000
C	4.049657000	4.328825000	1.177718000
C	2.908617000	5.086180000	1.382519000
C	1.908558000	5.098084000	0.408442000
C	2.165326000	4.465212000	-0.825753000
C	3.313933000	3.714257000	-1.041632000
C	0.485214000	5.379536000	0.427881000
C	-0.418734000	5.740476000	1.428353000
C	-1.767850000	5.478347000	1.254354000
C	-2.245611000	4.861033000	0.083340000
C	-1.377764000	4.649533000	-0.983494000
C	-0.024424000	4.900956000	-0.797432000
C	0.840765000	3.684650000	-2.792686000
C	-3.502465000	4.063820000	0.058943000
C	-3.687600000	3.183205000	1.118686000
C	-4.482888000	2.061301000	0.917445000

C	-5.117648000	1.808579000	-0.315657000
C	-5.060301000	2.789625000	-1.309141000
C	-4.259412000	3.901358000	-1.118055000
C	-5.429829000	0.390720000	-0.322460000
C	-4.971551000	-0.117624000	0.913075000
C	-4.710412000	-1.470928000	1.100441000
C	-4.871793000	-2.335866000	0.023742000
C	-5.473808000	-1.862945000	-1.160017000
C	-5.755153000	-0.518238000	-1.335470000
C	-3.721260000	0.736821000	2.888035000
C	-4.030903000	-3.564178000	0.047124000
C	-3.847511000	-4.324866000	1.217068000
C	-2.703770000	-5.081960000	1.408208000
C	-1.712788000	-5.088455000	0.425049000
C	-1.981055000	-4.449188000	-0.803323000
C	-3.131077000	-3.697231000	-1.005531000
C	-0.290298000	-5.373994000	0.426845000
C	0.623824000	-5.744092000	1.414949000
C	1.972126000	-5.488637000	1.226291000
C	2.439973000	-4.869168000	0.052044000
C	1.559889000	-4.648971000	-1.003158000
C	0.206942000	-4.890718000	-0.801838000
C	-0.686866000	-3.652466000	-2.777060000
N	4.737826000	-0.932472000	1.649315000
N	1.019254000	4.479258000	-1.601830000
N	-4.531979000	0.924570000	1.707816000
N	-0.844880000	-4.459845000	-1.591430000
H	3.286784000	-3.281412000	1.961358000
H	5.710396000	-2.636847000	-2.334305000
H	4.307904000	-4.626428000	-1.975275000
H	4.375971000	1.806638000	1.930116000
H	5.818286000	2.567116000	-2.031408000
H	6.296715000	0.175161000	-2.357780000
H	4.418072000	0.043009000	3.452519000
H	4.030788000	-1.675155000	3.452767000
H	4.784330000	4.241171000	1.969024000
H	2.759310000	5.591821000	2.329024000
H	3.403836000	3.085013000	-1.917729000
H	-0.063476000	6.141577000	2.370080000
H	-2.460734000	5.672947000	2.064042000
H	-1.722102000	4.109507000	-1.856234000
H	1.751912000	3.716788000	-3.387133000
H	0.034814000	4.107153000	-3.390572000
H	-3.057943000	3.261352000	1.995486000
H	-5.565787000	2.643564000	-2.256249000
H	-4.138274000	4.619387000	-1.919911000
H	-4.178029000	-1.808000000	1.980311000
H	-5.633546000	-2.554648000	-1.977920000
H	-6.137326000	-0.165351000	-2.285948000
H	-3.731178000	1.649903000	3.479991000
H	-2.689014000	0.484173000	2.623815000
H	-4.575868000	-4.242840000	2.014831000
H	-2.545960000	-5.592181000	2.350803000
H	-3.223701000	-3.060376000	-1.876127000
H	0.277383000	-6.147989000	2.358794000
H	2.673360000	-5.689931000	2.027087000

H	1.899086000	-4.112185000	-1.879623000
H	0.143794000	-4.036156000	-3.366638000
H	-0.502230000	-2.602493000	-2.527005000
H	-1.588730000	-3.722267000	-3.383112000
H	0.602160000	2.643328000	-2.551379000
H	-4.146047000	-0.060980000	3.494655000
H	2.930177000	-0.524935000	2.656002000
H	-3.181049000	-0.010071000	-0.900104000
Cl	-1.905068000	-0.021660000	-0.690055000

HBr@TCC

C	-2.147456000	4.866941000	0.114928000
C	-1.282797000	4.658579000	-0.955129000
C	0.071817000	4.904232000	-0.771109000
C	0.586400000	5.373892000	0.455531000
C	-0.313894000	5.732362000	1.460284000
C	-1.664359000	5.476168000	1.288090000
C	2.008628000	5.087021000	0.430870000
C	2.259602000	4.459779000	-0.807461000
C	3.403461000	3.703483000	-1.029918000
C	4.313318000	3.551200000	0.012014000
C	4.148218000	4.303980000	1.190195000
C	3.011488000	5.065808000	1.401958000
C	0.928236000	3.698846000	-2.777305000
C	5.141379000	2.313981000	-0.028610000
C	5.727406000	1.841621000	-1.218370000
C	5.985311000	0.493772000	-1.405792000
C	5.652225000	-0.414799000	-0.399471000
C	5.220281000	0.089976000	0.844604000
C	4.975649000	1.443011000	1.044107000
C	5.344433000	-1.832796000	-0.386850000
C	5.272417000	-2.816408000	-1.375294000
C	4.480976000	-3.932861000	-1.166449000
C	3.749350000	-4.096536000	0.025168000
C	3.957433000	-3.215705000	1.082001000
C	4.743773000	-2.091325000	0.862834000
C	4.060951000	-0.781251000	2.872351000
C	2.485768000	-4.883031000	0.071001000
C	1.603555000	-4.665654000	-0.983012000
C	0.250067000	-4.899413000	-0.775718000
C	-0.245953000	-5.371117000	0.457899000
C	0.669423000	-5.739793000	1.445370000
C	2.018427000	-5.492978000	1.250501000
C	-1.666714000	-5.077489000	0.458466000
C	-1.935452000	-4.445396000	-0.773531000
C	-3.082225000	-3.688772000	-0.977376000
C	-3.978351000	-3.543677000	0.076973000
C	-3.795467000	-4.298417000	1.251002000
C	-2.655069000	-5.059730000	1.444172000
C	-0.642089000	-3.677475000	-2.761120000
C	-4.814264000	-2.312051000	0.050092000
C	-5.407653000	-1.836004000	-1.136838000
C	-5.683077000	-0.490120000	-1.312981000
C	-5.359796000	0.417005000	-0.297947000
C	-4.909805000	-0.093650000	0.939120000

C	-4.656014000	-1.448046000	1.128005000
C	-5.038498000	1.832387000	-0.290781000
C	-4.970159000	2.812321000	-1.284759000
C	-4.162523000	3.918667000	-1.091256000
C	-3.408715000	4.076990000	0.088492000
C	-3.603860000	3.198362000	1.148099000
C	-4.406274000	2.081761000	0.944324000
C	-3.672068000	0.756626000	2.925706000
N	1.111922000	4.483407000	-1.580690000
N	4.812057000	-0.956840000	1.653818000
N	-0.801753000	-4.468581000	-1.565017000
N	-4.465899000	0.946038000	1.734661000
H	-1.631122000	4.125101000	-1.830246000
H	0.044982000	6.127100000	2.403332000
H	-2.354566000	5.669436000	2.100367000
H	3.487096000	3.077909000	-1.909289000
H	4.884793000	4.209187000	1.978901000
H	2.867320000	5.567578000	2.351329000
H	0.689133000	2.655865000	-2.543899000
H	1.837391000	3.734673000	-3.374668000
H	5.892304000	2.537125000	-2.032295000
H	6.355236000	0.142688000	-2.361721000
H	4.467324000	1.783915000	1.936889000
H	5.754495000	-2.668167000	-2.334243000
H	4.344618000	-4.650700000	-1.966139000
H	3.350211000	-3.297041000	1.974532000
H	4.506167000	0.021390000	3.457890000
H	4.111463000	-1.695135000	3.461595000
H	1.942210000	-4.136308000	-1.864214000
H	0.324003000	-6.135753000	2.392931000
H	2.721221000	-5.693121000	2.050213000
H	-3.174746000	-3.058749000	-1.852969000
H	-4.521706000	-4.208383000	2.049803000
H	-2.497436000	-5.564896000	2.389531000
H	0.176399000	-4.081730000	-3.354162000
H	-0.437442000	-2.628016000	-2.525114000
H	-5.566645000	-2.526774000	-1.955724000
H	-6.059213000	-0.135607000	-2.265306000
H	-4.129890000	-1.786867000	2.010967000
H	-5.473325000	2.669386000	-2.233616000
H	-4.034221000	4.635741000	-1.892850000
H	-2.975916000	3.270971000	2.026691000
H	-3.686428000	1.670631000	3.516353000
H	-2.637100000	0.499630000	2.676401000
H	-4.108325000	-0.038856000	3.527322000
H	3.011541000	-0.540833000	2.669907000
H	-1.550849000	-3.739356000	-3.357578000
H	0.120688000	4.127324000	-3.368738000
H	-3.064647000	-0.002703000	-0.919826000
Br	-1.685259000	0.008843000	-0.550692000

CH₄@TCC

C	5.124079000	-1.801402000	-0.021636000
C	4.870077000	-0.956467000	1.053522000
C	4.975867000	0.415104000	0.859413000

C	5.365736000	0.966776000	-0.377888000
C	5.790336000	0.100008000	-1.387580000
C	5.663209000	-1.267325000	-1.208512000
C	4.906829000	2.342606000	-0.367876000
C	4.265515000	2.532205000	0.873923000
C	3.363011000	3.567767000	1.085911000
C	3.078217000	4.427096000	0.029118000
C	3.833819000	4.340932000	-1.155926000
C	4.739316000	3.313376000	-1.357760000
C	3.688274000	1.147060000	2.865058000
C	1.746910000	5.092561000	0.066052000
C	1.212672000	5.643731000	1.245916000
C	-0.155281000	5.765072000	1.426637000
C	-1.022064000	5.326835000	0.423773000
C	-0.470913000	4.920742000	-0.809528000
C	0.900258000	4.810929000	-1.002037000
C	-2.408474000	4.898751000	0.405855000
C	-3.396197000	4.765477000	1.384202000
C	-4.445703000	3.886644000	1.175726000
C	-4.537355000	3.125629000	-0.005335000
C	-3.660133000	3.383306000	-1.054342000
C	-2.603439000	4.258245000	-0.835464000
C	-1.224925000	3.659535000	-2.826092000
C	-5.223895000	1.804545000	-0.042444000
C	-4.955679000	0.956715000	1.028083000
C	-5.060124000	-0.414493000	0.831579000
C	-5.449633000	-0.963305000	-0.407808000
C	-5.883845000	-0.095483000	-1.411812000
C	-5.766946000	1.272144000	-1.227200000
C	-5.003112000	-2.343841000	-0.394974000
C	-4.369990000	-2.538113000	0.850227000
C	-3.476926000	-3.580188000	1.066966000
C	-3.193418000	-4.441736000	0.011788000
C	-3.946710000	-4.354297000	-1.174549000
C	-4.843921000	-3.320026000	-1.380866000
C	-3.808235000	-1.166194000	2.855137000
C	-1.860421000	-5.104381000	0.051758000
C	-1.328972000	-5.658591000	1.231568000
C	0.038722000	-5.770944000	1.419278000
C	0.908058000	-5.320939000	0.423679000
C	0.361123000	-4.911348000	-0.810482000
C	-1.009808000	-4.810621000	-1.009815000
C	2.292594000	-4.887039000	0.414623000
C	3.276576000	-4.755478000	1.397101000
C	4.327927000	-3.877797000	1.193442000
C	4.426563000	-3.116292000	0.012998000
C	3.550895000	-3.369264000	-1.038467000
C	2.491723000	-4.242384000	-0.823798000
C	1.124103000	-3.633590000	-2.816166000
N	4.441957000	1.408225000	1.663084000
N	-1.470437000	4.405909000	-1.616914000
N	-4.542372000	-1.413331000	1.638730000
N	1.362418000	-4.387543000	-1.610015000
H	4.387770000	-1.349315000	1.939354000
H	6.127785000	0.490150000	-2.340413000
H	5.898555000	-1.938592000	-2.025528000

H	2.742005000	3.584059000	1.972615000
H	3.633348000	5.042839000	-1.956213000
H	5.244568000	3.217833000	-2.311404000
H	2.669181000	0.814944000	2.637280000
H	3.645341000	2.052513000	3.468037000
H	1.884670000	5.897717000	2.056659000
H	-0.545290000	6.117277000	2.374155000
H	1.296274000	4.326792000	-1.885374000
H	-3.298896000	5.274451000	2.335703000
H	-5.161858000	3.709888000	1.969010000
H	-3.682923000	2.758511000	-1.938123000
H	-0.923702000	2.628332000	-2.611621000
H	-0.439639000	4.150146000	-3.398417000
H	-4.477070000	1.350928000	1.915186000
H	-6.225803000	-0.484191000	-2.363610000
H	-6.012501000	1.945204000	-2.039690000
H	-2.858947000	-3.599518000	1.955657000
H	-3.749185000	-5.059227000	-1.972957000
H	-5.346346000	-3.223124000	-2.335891000
H	-4.311106000	-0.388262000	3.426856000
H	-2.778089000	-0.854488000	2.650841000
H	-2.003678000	-5.921363000	2.037238000
H	0.426141000	-6.126067000	2.366780000
H	-1.404718000	-4.323410000	-1.891864000
H	3.176030000	-5.266518000	2.347143000
H	5.042470000	-3.704338000	1.988890000
H	3.576923000	-2.744090000	-1.922051000
H	0.842145000	-2.598237000	-2.596447000
H	0.329058000	-4.109847000	-3.386892000
H	2.025231000	-3.636113000	-3.427409000
H	-2.128245000	3.649635000	-3.433757000
H	-3.795002000	-2.072191000	3.458792000
H	4.193944000	0.378853000	3.447401000
C	2.015088000	-0.022031000	-0.544369000
H	1.086320000	0.009903000	-1.112674000
H	1.962971000	-0.820260000	0.196068000
H	2.856210000	-0.213627000	-1.210830000
H	2.166832000	0.938647000	-0.050315000

C₂H₂@TCC

C	-3.215524000	4.306754000	0.036387000
C	-2.311825000	4.271485000	-1.023828000
C	-1.033354000	4.779831000	-0.826181000
C	-0.638348000	5.347442000	0.403327000
C	-1.604883000	5.525254000	1.394646000
C	-2.875806000	5.005982000	1.209795000
C	0.812031000	5.353334000	0.396957000
C	1.200540000	4.785153000	-0.833646000
C	2.476565000	4.275126000	-1.037551000
C	3.383823000	4.313846000	0.016766000
C	3.054251000	5.020284000	1.189179000
C	1.784512000	5.538062000	1.381773000
C	0.076125000	3.774974000	-2.822366000
C	4.449046000	3.273212000	-0.010368000
C	5.146003000	2.944136000	-1.188370000

C	5.682659000	1.681097000	-1.374873000
C	5.524513000	0.714998000	-0.379315000
C	4.968852000	1.107239000	0.855970000
C	4.442147000	2.377468000	1.054381000
C	5.521594000	-0.735678000	-0.379488000
C	5.675762000	-1.702143000	-1.375311000
C	5.134035000	-2.963072000	-1.189080000
C	4.436012000	-3.289719000	-0.011041000
C	4.432741000	-2.394181000	1.053913000
C	4.964417000	-1.125985000	0.855720000
C	3.979385000	-0.007750000	2.856096000
C	3.366876000	-4.326325000	0.016153000
C	2.459535000	-4.284119000	-1.037955000
C	1.181657000	-4.789373000	-0.833795000
C	0.791294000	-5.356090000	0.396913000
C	1.763307000	-5.544580000	1.381466000
C	3.034947000	-5.031638000	1.188581000
C	-0.659051000	-5.344715000	0.403622000
C	-1.052214000	-4.775813000	-0.825866000
C	-2.328869000	-4.262855000	-1.023379000
C	-3.232449000	-4.294473000	0.037057000
C	-2.895028000	-4.994645000	1.210561000
C	-1.626020000	-5.518687000	1.395208000
C	0.060285000	-3.775267000	-2.822410000
C	-4.308116000	-3.264415000	0.005190000
C	-4.978239000	-2.930734000	-1.187797000
C	-5.522600000	-1.672351000	-1.376557000
C	-5.397469000	-0.713765000	-0.369615000
C	-4.862108000	-1.106630000	0.873613000
C	-4.335084000	-2.377322000	1.077342000
C	-5.394650000	0.734398000	-0.369722000
C	-5.515848000	1.693238000	-1.376891000
C	-4.966355000	2.949457000	-1.188437000
C	-4.295101000	3.280799000	0.004553000
C	-4.325745000	2.394075000	1.076949000
C	-4.857709000	1.125387000	0.873451000
C	-3.860511000	0.007599000	2.862930000
N	0.080395000	4.572885000	-1.620150000
N	4.772908000	-0.009079000	1.651475000
N	0.062134000	-4.573006000	-1.620070000
N	-4.676051000	0.009080000	1.671865000
H	-2.543444000	3.689901000	-1.907695000
H	-1.343256000	5.988911000	2.338272000
H	-3.600080000	5.063526000	2.013130000
H	2.698639000	3.678070000	-1.912717000
H	3.784012000	5.079801000	1.987500000
H	1.528293000	6.004585000	2.325437000
H	0.958355000	4.012480000	-3.414232000
H	-0.802879000	4.022110000	-3.415379000
H	5.181039000	3.665520000	-1.995718000
H	6.138706000	1.422547000	-2.323041000
H	3.852185000	2.597503000	1.934884000
H	6.132716000	-1.445206000	-2.323480000
H	5.166062000	-3.684357000	-1.996643000
H	3.842123000	-2.612138000	1.934488000
H	4.224883000	0.872696000	3.447485000

H	4.222591000	-0.888571000	3.447893000
H	2.683658000	-3.687809000	-1.913116000
H	1.505526000	-6.010202000	2.325151000
H	3.764717000	-5.093984000	1.986676000
H	-2.558572000	-3.680622000	-1.907310000
H	-3.619264000	-5.049267000	2.014134000
H	-1.365945000	-5.983120000	2.338880000
H	0.942244000	-4.014856000	-3.413821000
H	0.056801000	-2.703208000	-2.597952000
H	-4.986542000	-3.645369000	-2.001775000
H	-5.955890000	-1.409086000	-2.334023000
H	-3.760168000	-2.596301000	1.968195000
H	-5.950070000	1.431500000	-2.334355000
H	-4.971572000	3.663871000	-2.002637000
H	-3.750177000	2.611108000	1.967856000
H	-4.092763000	0.888080000	3.459614000
H	-2.794742000	0.005851000	2.610557000
H	-4.095654000	-0.872238000	3.459418000
H	2.906761000	-0.006406000	2.634299000
H	-0.819009000	-4.020501000	-3.415802000
H	0.070333000	2.702965000	-2.597721000
H	-1.913066000	1.667374000	-0.342374000
C	-1.897289000	0.599973000	-0.345738000
C	-1.896345000	-0.598080000	-0.346029000
H	-1.910521000	-1.665501000	-0.343260000

C₂H₄@TCC

C	-0.546998000	-5.331182000	0.048606000
C	-1.220894000	-4.746413000	-1.019559000
C	-2.521642000	-4.301666000	-0.819925000
C	-3.178644000	-4.447215000	0.419833000
C	-2.550082000	-5.187303000	1.422624000
C	-1.247503000	-5.618697000	1.235188000
C	-4.276994000	-3.499184000	0.407428000
C	-4.209650000	-2.839522000	-0.836995000
C	-4.823396000	-1.611823000	-1.052394000
C	-5.506907000	-1.016395000	0.003647000
C	-5.721692000	-1.746788000	1.187671000
C	-5.116517000	-2.975551000	1.392648000
C	-2.726434000	-2.856543000	-2.842731000
C	-5.582917000	0.470680000	-0.032591000
C	-5.858044000	1.180023000	-1.217097000
C	-5.383263000	2.466744000	-1.409366000
C	-4.613496000	3.070205000	-0.413070000
C	-4.488083000	2.413407000	0.828445000
C	-4.974851000	1.128628000	1.032708000
C	-3.618670000	4.126698000	-0.411388000
C	-3.065131000	4.936609000	-1.404362000
C	-1.813638000	5.495812000	-1.206468000
C	-1.090778000	5.266237000	-0.020901000
C	-1.706073000	4.607595000	1.039511000
C	-2.956359000	4.038604000	0.830758000
C	-3.026048000	2.565782000	2.843137000
C	0.396140000	5.326465000	0.020315000
C	1.058465000	4.712896000	-
			1.038732000

C	2.357969000	4.263829000	-0.839493000
C	3.023612000	4.431954000	0.393071000
C	2.403397000	5.189516000	1.388274000
C	1.103169000	5.626748000	1.200133000
C	4.129040000	3.493270000	0.384490000
C	4.063068000	2.822357000	-0.854045000
C	4.690677000	1.599892000	-1.063986000
C	5.374735000	1.014454000	-0.003237000
C	5.578674000	1.751211000	1.179864000
C	4.967141000	2.977890000	1.376223000
C	2.552833000	2.769480000	-2.832492000
C	5.457466000	-0.472445000	-0.027780000
C	5.720265000	-1.187441000	-1.213211000
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C	4.858615000	-1.124477000	1.045097000
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C	1.544041000	-4.567600000	1.057250000
C	2.795601000	-4.000427000	0.848814000
C	2.859085000	-2.482915000	2.832411000
N	-3.239899000	-3.434932000	-1.625873000
N	-3.588362000	3.098750000	1.627276000
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N	3.432069000	-3.059526000	1.639481000
H	-0.672370000	-4.466897000	-1.910020000
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H	2.752107000	-0.864702000	-0.773281000
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H	0.918269000	-1.090690000	-0.695145000
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H	0.742396000	0.877166000	0.779021000

C₂H₆@TCC

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C	1.462173000	4.697268000	-1.024867000
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C	2.875256000	2.731130000	-2.837374000
C	5.556467000	-0.729205000	-0.021478000
C	5.802507000	-1.446196000	-1.207738000
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