

Electronic Supplementary Information

Theoretical Investigation of C1-C4 Hydrocarbons Adsorption and Separation in a Porous Metallocavitand

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Table S1: Bond length (Å) of pristine hydrocarbon guest and the encapsulated guest.

HC@PPX	BLG@PPX (Å)	BLPG(Å)
CH₄@PPX	C–H: 1.104	C–H: 1.101
C₂H₂@PPX	C≡C: 1.231, C–H: 1.073	C≡C: 1.230, C–H: 1.073
C₂H₄@PPX	C=C: 1.354, C–H: 1.094	C=C: 1.355, C–H: 1.094
C₂H₆@PPX	C–C: 1.548, C–H: 1.103	C–C: 1.552, C–H: 1.103
Allene@PPX	C=C: 1.323, C–H: 1.090	C–C: 1.330, C–H: 1.094
C₃H₄@PPX	C–C: 1.470, C≡C: 1.230, C–H: 1.101	C–C: 1.477, C≡C: 1.232, C–H: 1.103
C₃H₆@PPX	C–C: 1.514, C=C: 1.357, C–H: 1.104	C–C: 1.518, C=C: 1.357, C–H: 1.102
C₃H₈@PPX	C–C: 1.547, C–H: 1.103	C–C: 1.551, C–H: 1.104
1,2-butadiene	C–C: 1.525, C=C: 1.327, C–H: 1.096, C–H: 1.106	C–C: 1.528, C=C: 1.331, C–H: 1.097 C–H: 1.100
1,3-butadiene	C–C: 1.463, C=C: 1.362, C–H: 1.094	C–C: 1.468, C=C: 1.364, C–H: 1.096
1-Buynes	C–C: 1.557, C–C: 1.476, C≡C: 1.230 C–H: 1.069, C–H: 1.104	C–C: 1.560, C–C: 1.480, C≡C: 1.232, C–H: 1.071, C–H: 1.104
2-Buynes	C–C: 1.472, C≡C: 1.230, C–H: 1.105	C–C: 1.478, C≡C: 1.233, C–H: 1.104
C₄H₈@PPX	C–C: 1.550, C=C: 1.355, C–H: 1.103	C–C: 1.558, C=C: 1.356, C–H: 1.103
(E)-C₄H₈@PPX	C–C: 1.515, C=C: 1.357, C–H: 1.103	C–C: 1.519, C=C: 1.357, C–H: 1.104
(Z)-C₄H₈@PPX	C–C: 1.517, C=C: 1.359, C–H: 1.103	C–C: 1.519, C=C: 1.360, C–H: 1.104
Isobutylene@PPX	C–C: 1.517, C=C: 1.356, C–H: 1.102	C–C: 1.523, C=C: 1.358, C–H: 1.104
C₄H₁₀@PPX	C–C: 1.545, C–H: 1.107	C–C: 1.550, C–H: 1.106
Iso-butane@PPX	C–C: 1.542, C–H: 1.101	C–C: 1.551, C–H: 1.104

HC@PPX: Hydrocarbon encapsulated Pillarplex host

BLG@PPX: Bond length of hydrocarbon encapsulated pillarplex

BLPG: Bond length of the pristine guest

Table S2: The Au-Au and N \cdots H-C bond length in Å of PPX and HC@PPX.

HC@PPX	Au-Au bond distance (Å)	N\cdotsH-C bond distance (Å)
CH₄@PPX	3.141	2.884
C₂H₂@PPX	3.150	2.582
C₂H₄@PPX	3.156	2.807
C₂H₆@PPX	3.148	2.819
Allene@PPX	3.209	2.427
C₃H₄@PPX	3.154	2.616
C₃H₆@PPX	3.125	2.676
C₃H₈@PPX	3.144	2.611
1,2-butadiene	3.132	2.591
1,3-butadiene	3.141	2.687
1-Buynne	3.128	2.735
2-Buynne	3.123	2.891
C₄H₈@PPX	3.150	2.547
(E)-C₄H₈@PPX	3.109	2.714
(Z)-C₄H₈@PPX	3.198	2.681
Isobutylene@PPX	3.170	2.766
C₄H₁₀@PPX	3.138	2.621
Isobutane@PPX	3.245	2.348

Table S3: Deformation energy of the guest molecule, charge transfer from guest hydrocarbon to PPX host, electronic charge transfers from Au atom, change in enthalpy (ΔH), and change in entropy (ΔS).

Gas Molecules	Deformation Energy of Guest (kcal/mol)	Charge transfer G→H (e ⁻)	Charge transfer from Au (e ⁻)	ΔS (kcal/mol* kelvin)
CH ₄	0.023	0.052	0.015	-0.028
C ₂ H ₂	0.002	0.045	0.015	-0.022
C ₂ H ₄	0.014	0.072	0.019	-0.038
C ₂ H ₆	0.052	0.096	0.021	-0.039
Allene	0.201	0.075	0.013	-0.045
C ₃ H ₄	0.112	0.075	0.014	-0.041
C ₃ H ₆	0.122	0.108	0.023	-0.041
C ₃ H ₈	0.185	0.119	0.026	-0.044
1,2-butadiene	0.105	0.099	0.021	-0.042
1,3-butadiene	0.085	0.105	0.023	-0.042
1-butyne	0.033	0.093	0.024	-0.042
2-butyne	0.138	0.070	0.013	-0.043
C ₄ H ₈	0.594	0.118	0.024	-0.046
(E)-C ₄ H ₈	0.122	0.113	0.025	-0.045
(Z)-C ₄ H ₈	0.133	0.119	0.025	-0.044
Isobutylene	0.181	0.115	0.021	-0.050
C ₄ H ₁₀	0.172	0.129	0.028	-0.046
Isobutane	0.786	0.129	0.019	-0.052

Table S4: Energy decomposition analysis of HC@PPX represents electrostatic energy (ΔE_{elct}), dispersion energy (ΔE_{disp}), orbital energy (ΔE_{orb}), and Pauli's repulsion (ΔE_{pau}). The energy values are given in the kcal/mol unit. The percentage of contribution of each attractive term is given in the parenthesis.

Gas Molecules	ΔE_{elct} (kcal/mol)	ΔE_{disp} (kcal/mol)	ΔE_{orb} (kcal/mol)	ΔE_{Pau} (kcal/mol)
CH₄	-4.6 (22.5)	-12.4 (61.4)	-3.3 (16.1)	9.7
C₂H₂	-7.5 (25.1)	-16.4 (54.8)	-6.0 (20.1)	15.8
C₂H₄	-8.7 (24.7)	-19.9 (56.2)	-6.8 (19.1)	20.7
C₂H₆	-11.8 (28.3)	-22.6 (54.0)	-7.4 (17.7)	25.7
Allene	-19.9 (34.3)	-26.6 (45.8)	-11.5 (19.9)	41.6
C₃H₄	-15.0 (30.1)	-25.8 (51.9)	-9.0 (18.0)	31.8
C₃H₆	-14.2 (28.0)	-27.9 (55.2)	-8.5 (16.8)	28.4
C₃H₈	-16.2 (28.8)	-30.2 (53.7)	-9.9 (17.5)	33.8
1,2-butadiene	-17.2 (29.2)	-32.8 (55.7)	-8.9 (15.1)	34.3
1,3-butadiene	-16.2 (27.6)	-32.5 (55.5)	-10.0 (16.9)	34.8
1-butyne	-13.8 (25.5)	-30.8 (57.0)	-9.5 (17.5)	30.6
2-butyne	-14.1 (26.3)	-31.1 (58.3)	-8.1 (15.4)	29.4
C₄H₈	-19.2 (30.1)	-34.3 (53.5)	-10.5 (16.4)	39.1
(E)-C₄H₈	-16.2 (26.0)	-36.2 (58.2)	-9.8 (15.8)	34.5
(Z)-C₄H₈	-17.8 (27.9)	-36.1 (56.6)	-9.9 (15.5)	34.5
Isobutylene	-24.4 (32.6)	-36.5 (48.8)	-13.9 (18.6)	49.2
C₄H₁₀	-19.0(27.7)	-37.8 (55.1)	-11.8 (17.2)	40.8
Isobutane	-26.8 (34.0)	-37.8 (47.9)	-14.2 (18.1)	57.9

Table S5. Uptake of C1-C3 HCs on various materials at 298 K temperature and 1 bar pressure.

For those ambient conditions data is not available the nearest conditions are considered.

Host	Hydrocarbons							Cond.	Ref.
	CH ₄	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆	C ₃ H ₄	C ₃ H ₆	C ₃ H ₈		
Ni ₂ (BTEC)(bipy) ₃		3.42	0.35					298/1	[93]
PCN-250/MIL-100		4.5/2.0						295/0.7	[94]
PCN-207-FA	0.82	3.07	2.27	2.37		2.17		273/ 1	[85]
UPC-98	0.26	1.35	0.79	2.03		5.2	4.34	298/1	[69]
UMCM-151/UMCM-151-F/-Cl/-NH ₂ /-CH ₃ /-OCH ₃		2.22/4.40/ 4.03/3.91/ 3.33/3.57	2.68/3.22/ 3.01/4.37/ 4.03/4.20	2.31/3.05/ 2.99/3.69/ 3.47/3.55		3.07/4.72/ 4.29/4.88/ 4.61/4.48	2.98/4.36/ 3.96/4.48/ 4.47/4.11	273/1	[70]
PFC-5		1.37	1.17	1.15				298/1	[71]
Mg-MOF-74/tpt-Mg-MOF-74				6.1/5.4			6.6/6.1	298/1	[66]
MFM-300(In)		4.5	4.9	5.1	6.3	5.4	4.8	293/ 1	[81]
MOF-801						3.5	3.2	303/1	[86]
NKM-101a		3.75	2.90	2.92			3.34	298/1	[92]
FIR-125/126	0.54/0.74	1.69/2.59	1.33/2.12	1.42/1.88			1.36/1.52	298/1	[72]
ZJNU-120-Sm	0.47	3.07	2.36	2.80				298/1	[95]
NOTT-101/-IPA	5.93/5.98							298/5	[68]
PAN-p1/-m1/ -m2/-m3	0.91/0.62/ 0.72/0.71			3.75/2.53/ 2.63/2.71			5.11/3.42/ 3.55/4.01	298/1	[96]
Ni(TMBDC)(DABCO) _{0.5}	0.4			5.81			5.54	298/1	[97]
NUM-9a		2.32	2.36	2.48				298/1	[73]
Zr-OBBA/-SDBA/ JLU-Liu45	0.15/0.56/ 0.69	0.99/4.51/ 2.52	0.54/1.82/ 1.99	0.5/2.07/ 3.78			0.78/2.45/ 3.79	298/1	[74]
PFC-1/-2	0.30/0.48	1.27/2.13	1.30/1.83					298/1	[75]
Cu-CPAH	1.28	5.88						298/1	[98]
NUM-7		2.47	2.61	2.85				298/1	[76]
PAN-5H/-5F/ -2F/-2(CF ₃)	0.59/0.33/ 0.76/0.75		2.25/1.25/ 3.20/3.10	2.35/1.30/ 3.64/3.53			3.63/1.93/ 4.62/4.60	298/1	[99]
Gly@HKUST-1s	0.9			6.47			7.80	298/1	[100]
UTSA-220	0.59	3.40	2.53	2.14				298/1	[101]
Cu-F-pymo		0.10						298/1	[77]
Dps-VCo-BDC/tpt-VCo-BDC	1.07/1.29	10.44/7.85	7.41/6.29	8.03/6.69				298/1	[82]
MOF 1/MOF 2	0.26/0.17	1.07/3.48	0.66/1.74	0.49/1.74				298/1	[78]
UPC-99	0.44	1.92	1.98	2.72		5.33	4.85	298/1	[79]
BSF-2	0.29			1.52			2.21	298/1	[102]
NPU-1/-2/-3		5.1/4.03/ 2.58	4.2/3.45/ 2.22	4.5/4.44/ 3.36				298/1	[84]
NbU-1		2.72	1.65	1.56				298/1	[80]
PPX	2.37	2.80	4.26	4.22	3.60	3.57	3.12	298/1	This work

Table S6: A brief comparison of C4 uptake by PPX and other reported systems. The values are in the range of mmol g^{-1} in the ambient conditions. For those ambient condition data is unavailable, the nearest temperature and pressures are on account.

Host	(E)-C ₄ H ₈	(Z)-C ₄ H ₈	1,3- butadiene	C ₄ H ₈	isobutylene	C ₄ H ₁₀	isobutane	Cond.
M-Gallate (M	1.09/1.85/	0.44/0.58/	1.39/1.96/	0.57/1.46/	0.09/0.13/	0.08/0.17/	0.07/0.08/	
=Ni/Mg/Co)	1.67	0.58	1.86	0.88	0.13	0.31	0.10	298/1
ZU-36-Co				2.35	0.17	2.20	0.12	298/1
FJI-H19	7.53	7.26				7.53	7.72	295/1
TMOF-1/ZU-619			1.64/1.58	1.08/0.63	0.20/0.30			298/1
M₂(dobdc)	0.77/0.91/	0.27/0.29/		0.24/0.24/				
(M=Mn/Fe/Co/Ni)	1.17/1.19	0.46/0.39		0.34/0.34				328/1
M₂(m-dobdc)	0.51/0.71/	0.14/0.19/		0.12/0.12/				
(M=Mn/Fe/Co/Ni)	0.83/0.70	0.24/0.16		0.14/0.10				328/1
NKM-101a			3.54			3.08	2.54	298/1
PPX	2.50	2.60	2.95	2.50	2.4	2.32	1.93	298/1

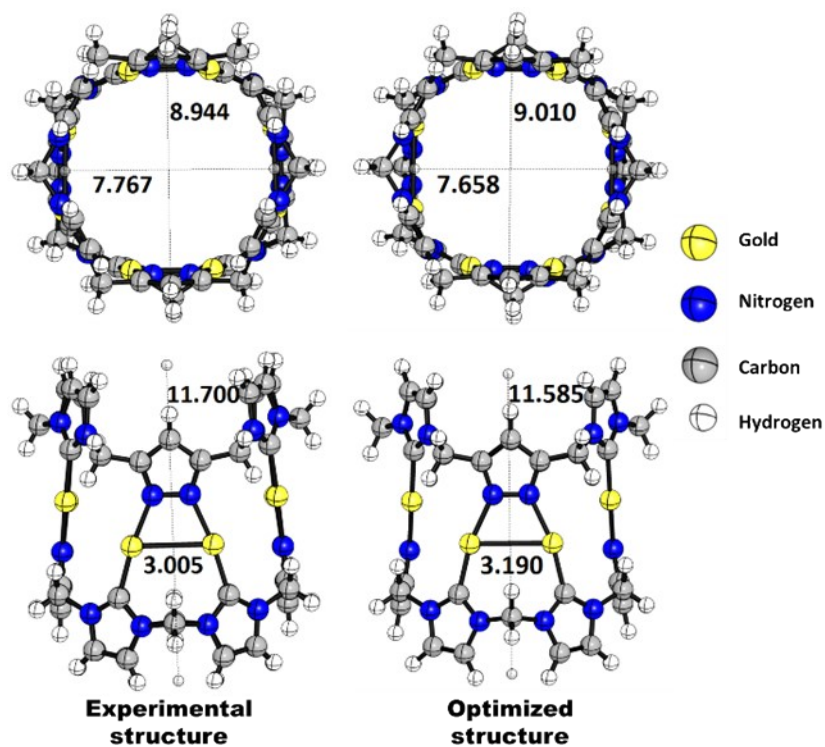


Figure S1: Height, width and Au-Au bond length of experimental and optimized pillarplex (PPX) geometry.

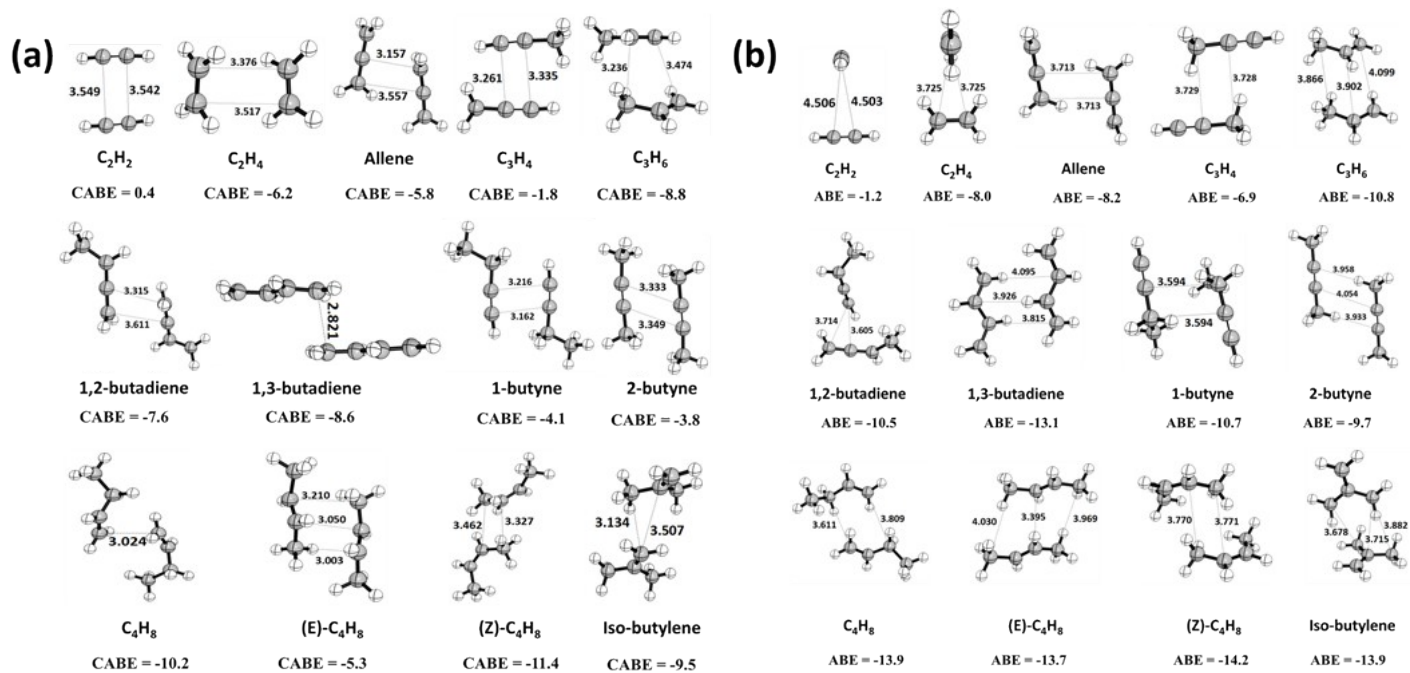


Figure S2: The constrained dimer (a) and relax dimer (b) structure of HCs and their corresponding C-C bond distance, cooperative adsorption binding energy (CABE) and adsorption binding energy (ABE). The bond distances are given in Å unit and the energy terms are in kcal/mol.

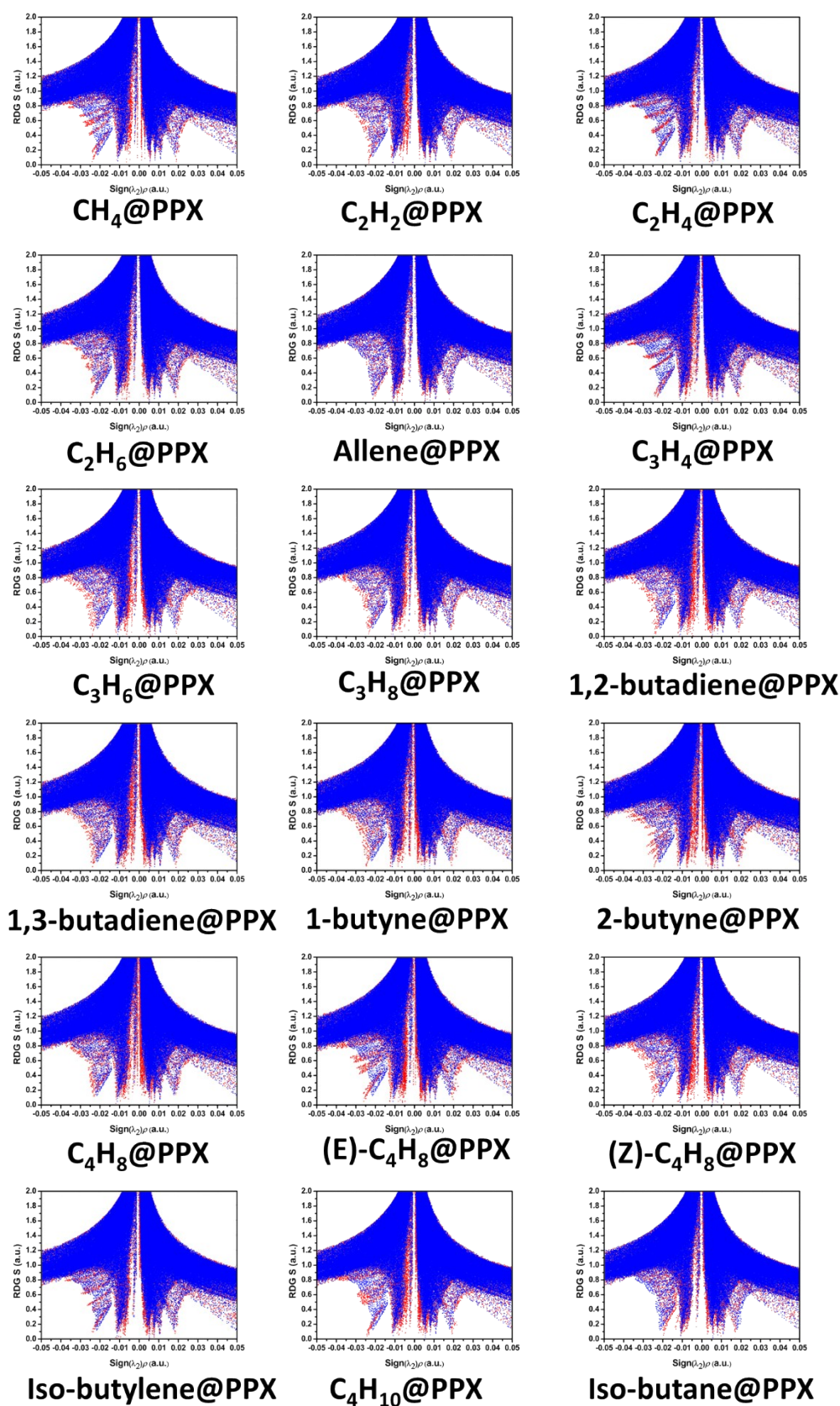


Figure S3: The superimposed NCI-RDG image of PPX and HC@PPX. The red and blue colour represents HC@PPX and pristine PPX respectively.

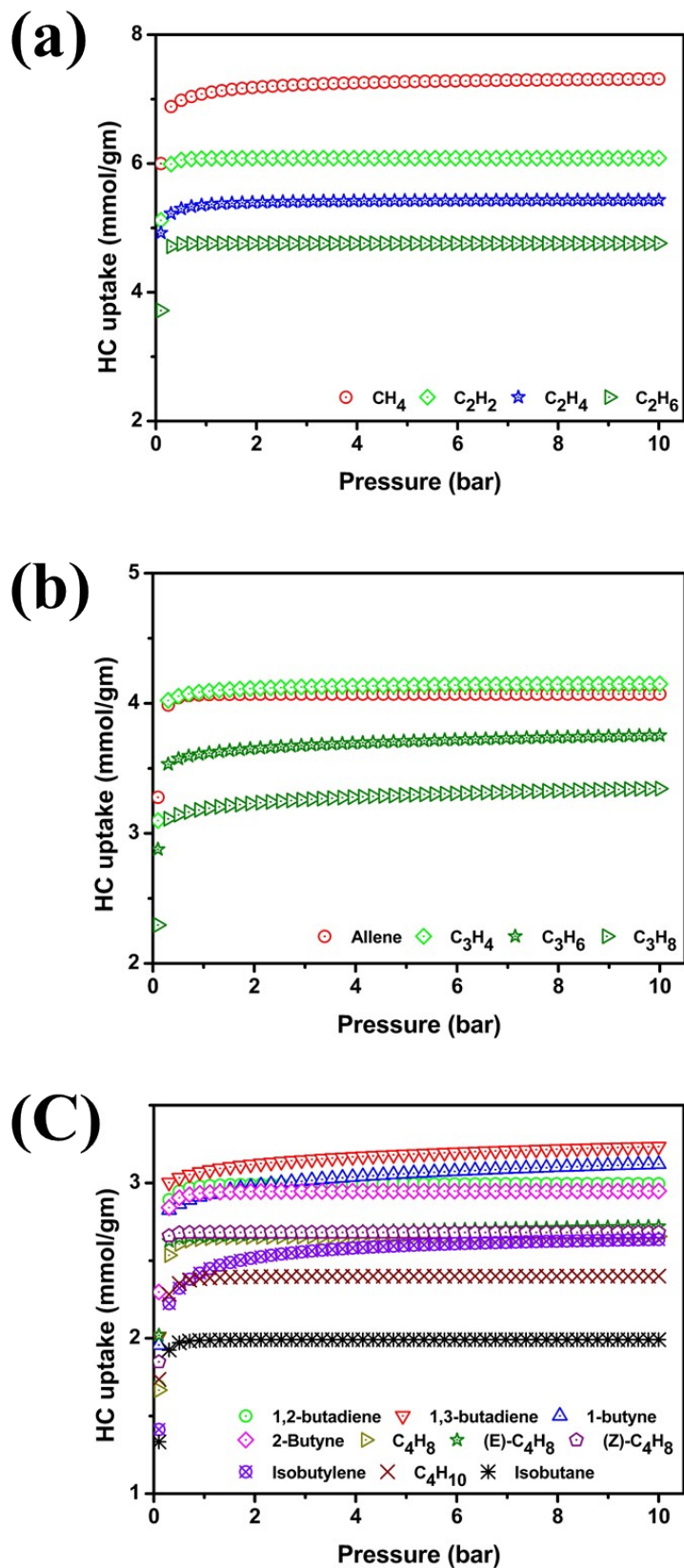


Figure S4: Grand canonical Monte Carlo simulation of (a) C1/C2, (b) C3 and (c) C4 with PPX at 77 K and 0.1-10 bar pressure.

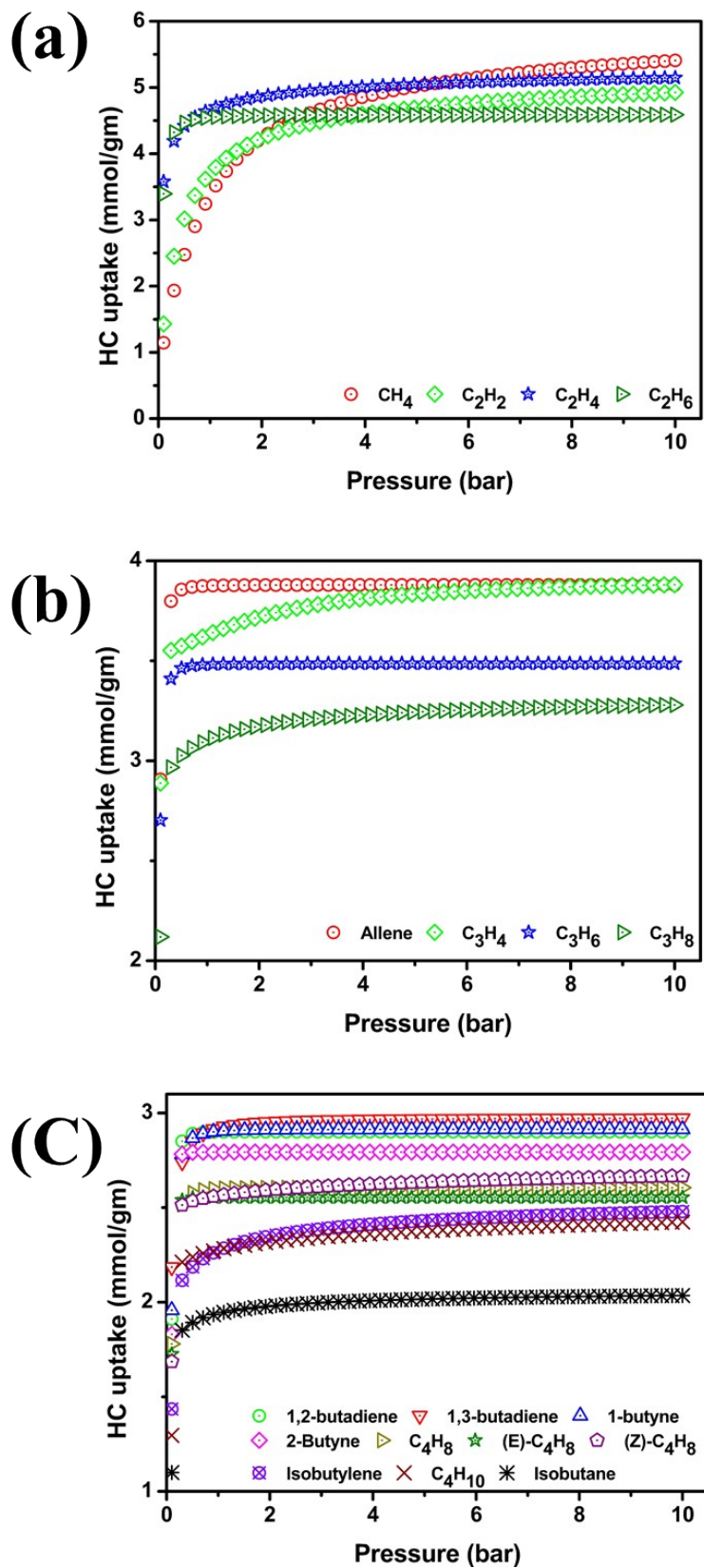


Figure S5: Grand canonical Monte Carlo simulation of (a) C1/C2, (b) C3 and (c) C4 with PPX at 273 K and 0.1-10 bar pressure.

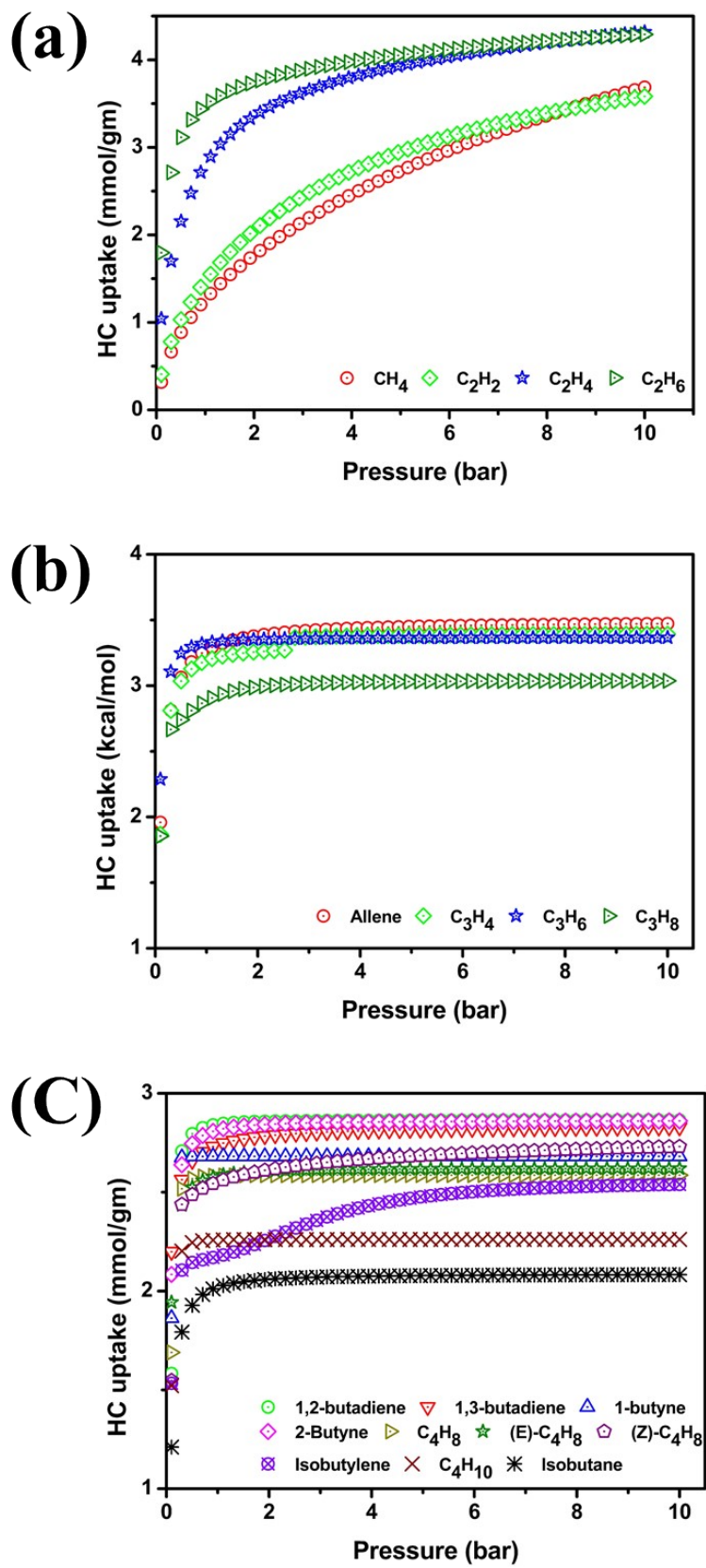


Figure S6: Grand canonical Monte Carlo simulation of (a) C1/C2, (b) C3 and (c) C4 with PPX at 340 K and 0.1-10 bar pressure.

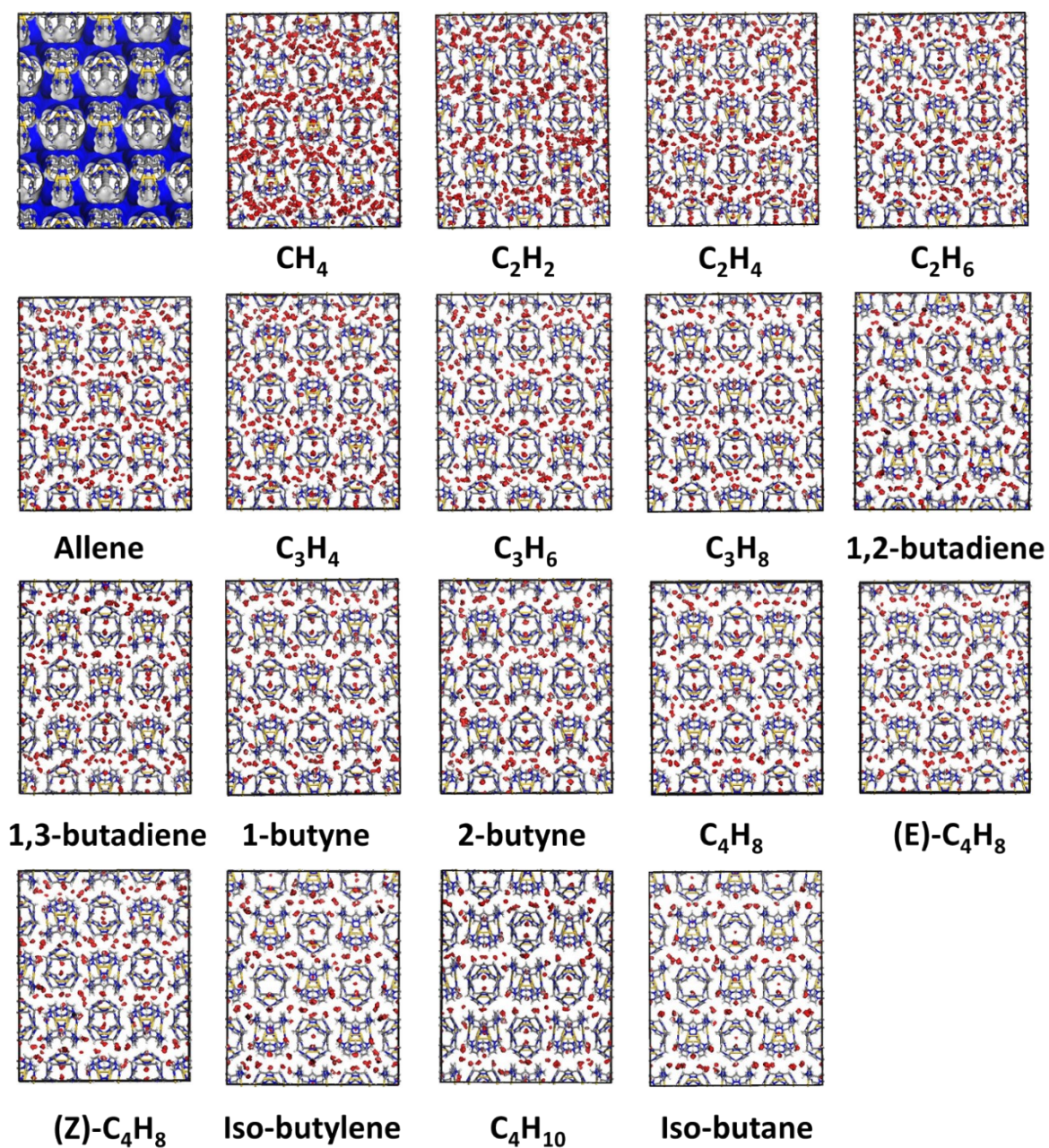


Figure S7. Pore surface of PPX and density distribution plot of HCs adsorbed PPX obtained from GCMC simulation at 298 K temperature and 1 bar pressure.

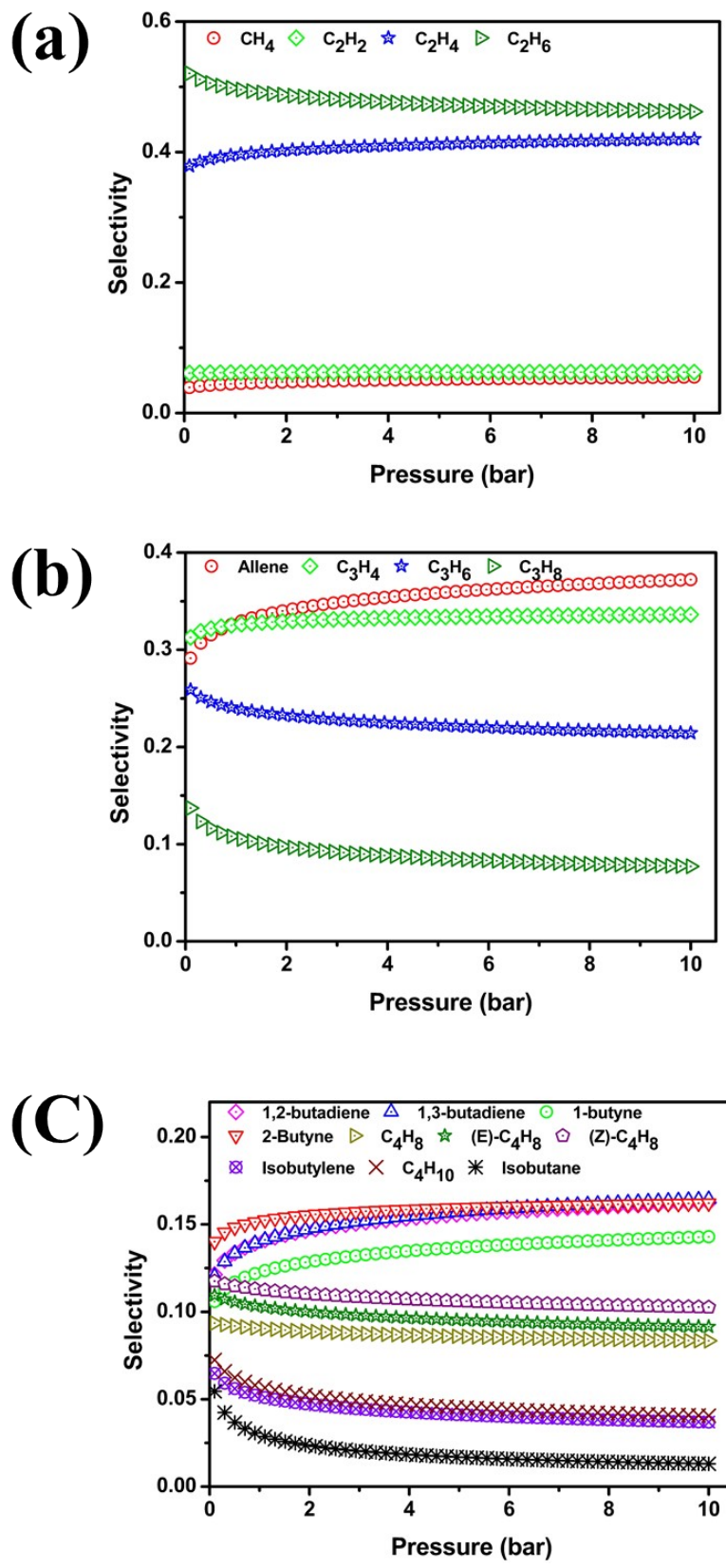


Figure S8: Ideal adsorption solution theory for separation of (a) C1/C2, (b) C3 and (c) C4 hydrocarbons from their isomers at 273 K.

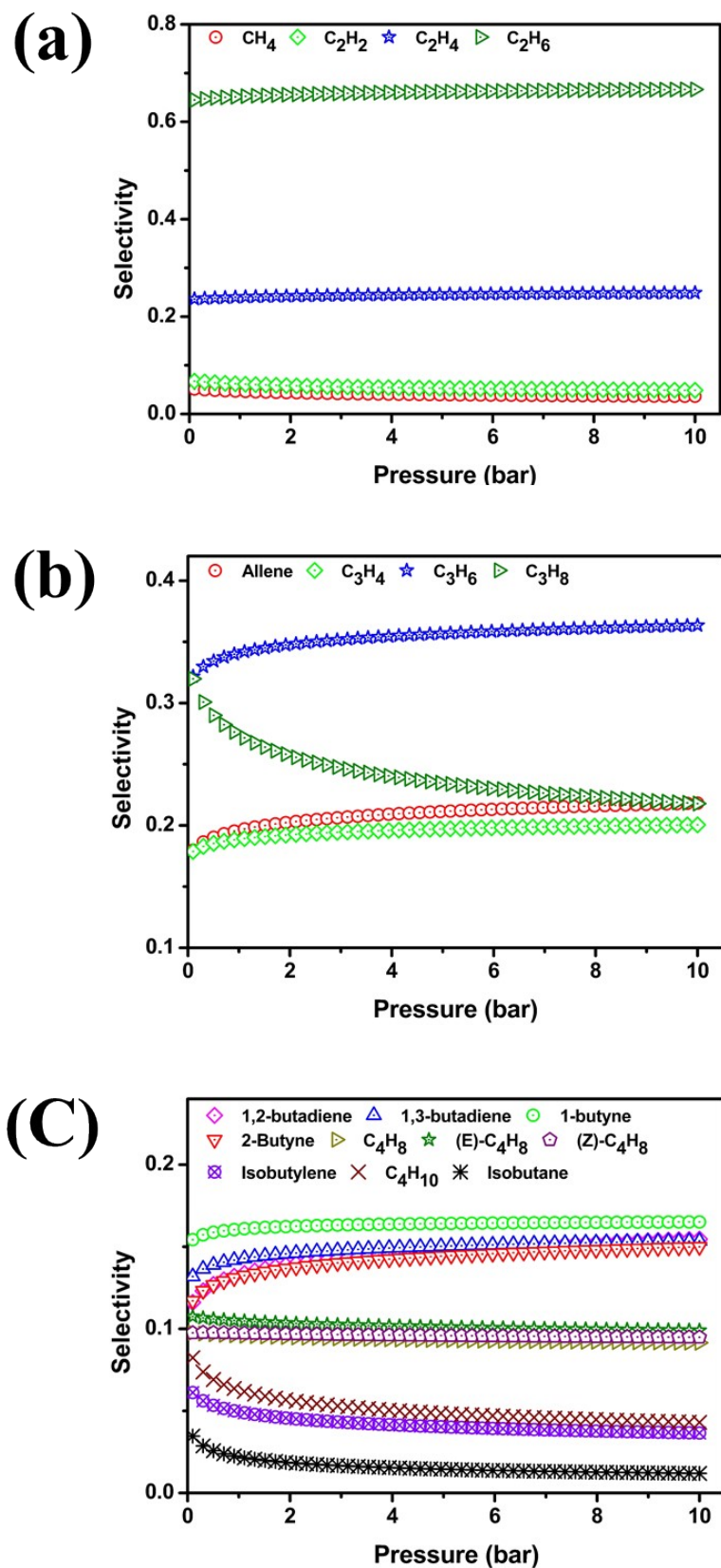


Figure S9: Ideal adsorption solution theory for separation of (a) C1/C2, (b) C3 and (c) C4 hydrocarbons from their isomers at 340 K.

Coordinates

CH₄@PPX

Au	-1.575720000	-3.660620000	-0.834348000	C	-1.879679000	-3.913235000	-5.069875000
Au	1.567043000	-3.653994000	-0.829148000	C	0.003100000	-4.897232000	-3.650195000
Au	3.902769000	-1.570521000	0.841814000	C	2.049810000	-3.654754000	-2.777649000
Au	-3.920677000	-1.568506000	0.829419000	C	3.101362000	-3.313958000	-4.792549000
Au	-1.569544000	3.663056000	-0.834298000	C	1.893466000	-3.918600000	-5.062663000
Au	1.573181000	3.651038000	-0.829098000	C	-4.335266000	-2.594217000	-2.665093000
Au	3.906010000	1.564709000	0.841873000	C	-4.196729000	-1.123711000	-2.365408000
Au	-3.918196000	1.574760000	0.829466000	C	4.341863000	-2.601775000	-2.649880000
N	-3.171025000	-3.163801000	-3.406899000	C	4.209562000	-1.130288000	-2.352879000
N	-1.247207000	-4.123811000	-3.826256000	C	3.788231000	-2.030046000	2.792138000
N	1.254029000	-4.123711000	-3.821631000	C	3.933505000	-1.857661000	5.086225000
N	3.177864000	-3.166845000	-3.395389000	C	3.277171000	-3.033315000	4.795471000
N	-4.007228000	-0.696498000	-1.073987000	C	2.584615000	-4.246674000	2.632613000
N	4.017993000	-0.702497000	-1.062388000	C	1.116510000	-4.055416000	2.345406000
N	4.240101000	-1.246957000	3.851958000	C	-0.012673000	-4.250923000	3.174227000
N	3.200735000	-3.119418000	3.393406000	C	-1.139144000	-4.052573000	2.342522000
N	0.691447000	-3.744164000	1.076310000	C	-2.608573000	-4.242004000	2.625832000
N	-0.709041000	-3.742927000	1.074259000	C	-3.815854000	-2.026361000	2.780223000
N	-3.226917000	-3.113787000	3.383953000	C	-3.960049000	-1.848001000	5.073789000
N	-4.267070000	-1.240271000	3.838123000	C	-3.303178000	-3.024085000	4.785826000
N	-3.165599000	3.168804000	-3.406898000	C	-2.041341000	3.660041000	-2.785111000
N	-1.240191000	4.125678000	-3.826198000	C	-3.081931000	3.311444000	-4.804073000
N	1.261076000	4.121900000	-3.821507000	C	-1.872989000	3.916178000	-5.069828000
N	3.183537000	3.162242000	-3.395348000	C	0.011261000	4.897204000	-3.650022000
N	-4.006049000	0.702951000	-1.073978000	C	2.056115000	3.651550000	-2.777573000
N	4.019363000	0.696603000	-1.062386000	C	3.107399000	3.309903000	-4.792471000
N	4.242252000	1.240138000	3.851998000	C	1.900363000	3.916283000	-5.062528000
N	3.206047000	3.114359000	3.393486000	C	-4.330848000	2.601223000	-2.665118000
N	0.697706000	3.742669000	1.076383000	C	-4.194839000	1.130495000	-2.365400000
N	-0.702803000	3.743742000	1.074336000	C	4.346638000	2.595255000	-2.649901000
N	-3.221764000	3.118856000	3.383979000	C	4.211747000	1.124008000	-2.352887000
N	-4.265004000	1.247055000	3.838147000	C	3.792020000	2.024192000	2.792202000
C	-2.047585000	-3.656917000	-2.785137000	C	3.936240000	1.851085000	5.086289000
C	-3.087629000	-3.306545000	-4.804078000	C	3.281836000	3.027825000	4.795558000

C	2.591646000	4.242541000	2.632695000	H	-4.420625000	3.158188000	-1.721422000
C	1.123263000	4.053430000	2.345466000	H	-5.227520000	2.790962000	-3.272582000
C	-0.005616000	4.250816000	3.174249000	H	5.245498000	2.788054000	-3.253102000
C	-1.132398000	4.054182000	2.342571000	H	4.431029000	3.150334000	-1.704551000
C	-2.601522000	4.246059000	2.625864000	H	4.233184000	1.432825000	6.040194000
C	-3.812556000	2.032432000	2.780254000	H	2.908283000	3.803978000	5.451854000
C	-3.956778000	1.854162000	5.073816000	H	2.750751000	5.158325000	3.219960000
C	-3.298009000	3.029185000	4.785851000	H	3.140389000	4.332709000	1.684430000
C	-4.317406000	0.003496000	-3.210499000	H	-0.006754000	4.539382000	4.220358000
C	4.335005000	-0.003263000	-3.197849000	H	-3.147380000	4.338638000	1.676215000
C	5.032436000	-0.004090000	3.712687000	H	-2.759891000	5.161680000	3.213561000
C	-5.057033000	0.004053000	3.695893000	H	-4.255520000	1.435053000	6.026771000
H	-3.885215000	-3.007175000	-5.472748000	H	-2.921867000	3.802438000	5.444080000
H	-1.450971000	-4.235717000	-6.010805000	H	-4.505038000	0.003652000	-4.279143000
H	0.004590000	-5.705332000	-4.394250000	H	4.525019000	-0.003457000	-4.266051000
H	0.001249000	-5.325134000	-2.641996000	H	5.504740000	-0.004485000	2.724467000
H	3.903141000	-3.018650000	-5.458003000	H	5.804333000	-0.004786000	4.493993000
H	1.468893000	-4.243247000	-6.004724000	H	-5.525403000	0.004458000	2.705792000
H	-4.425920000	-3.151009000	-1.721373000	H	-5.831696000	0.004686000	4.474470000
H	-5.232297000	-2.782454000	-3.272496000	H	2.902688000	-3.809050000	5.451733000
H	5.240432000	-2.796096000	-3.253031000	C	0.346860000	-0.000648000	-0.115216000
H	4.425306000	-3.156972000	-1.704524000	H	0.045446000	0.905284000	-0.670297000
H	4.231498000	-1.440099000	6.040108000	H	-0.148540000	0.000106000	0.869509000
H	2.742393000	-5.162700000	3.219856000	H	0.046755000	-0.908251000	-0.668233000
H	3.133188000	-4.337647000	1.684329000	H	1.439724000	0.000375000	0.022650000
H	-0.014263000	-4.539270000	4.220392000	<u>C₂H₂@PPX</u>			
H	-3.154619000	-4.333647000	1.676198000	Au	4.288799000	0.665033000	0.844253000
H	-2.768463000	-5.157365000	3.213524000	Au	3.460840000	-2.374683000	0.835997000
H	-4.258162000	-1.428427000	6.026738000	Au	0.661137000	-3.819948000	-0.827648000
H	-2.928338000	-3.797968000	5.444056000	Au	2.423092000	3.175814000	-0.825100000
H	-3.880008000	3.013437000	-5.472768000	Au	-3.461385000	2.374936000	0.835760000
H	-1.443770000	4.238022000	-6.010743000	Au	-4.289394000	-0.664740000	0.844322000
H	0.013975000	5.705390000	-4.393980000	Au	-2.422831000	-3.175786000	-0.824856000
H	0.010016000	5.325011000	-2.641783000	Au	-0.660927000	3.819103000	-0.827967000
H	3.908822000	3.013634000	-5.457927000	N	3.896009000	2.313408000	3.397202000
H	1.476327000	4.241782000	-6.004535000	N	4.470226000	0.250214000	3.855425000

N	3.861177000	-2.157528000	3.847492000	C	3.602152000	-3.464701000	-2.657493000
N	2.391385000	-3.712392000	3.378453000	C	3.848318000	-2.008726000	-2.357582000
N	1.584271000	3.444048000	1.081105000	C	4.241660000	-0.946248000	-3.204158000
N	-0.215461000	-3.738269000	1.077695000	C	4.426654000	0.169681000	-2.357207000
N	0.242179000	-4.223971000	-3.816755000	C	4.906000000	1.565522000	-2.660761000
N	2.333502000	-3.722149000	-3.399622000	C	2.893140000	3.083678000	-2.775489000
N	3.796501000	-1.554853000	-1.063552000	C	2.790211000	3.385615000	-5.058689000
N	4.156532000	-0.200917000	-1.062217000	C	3.849174000	2.545161000	-4.795249000
N	3.896214000	2.378871000	-3.399051000	C	-3.231645000	2.800062000	2.783095000
N	2.208081000	3.710085000	-3.814905000	C	-2.482717000	3.653512000	4.780531000
N	-2.391284000	3.712657000	3.378003000	C	-3.408623000	2.678141000	5.078100000
N	-3.861311000	2.158092000	3.847286000	C	-4.936450000	1.148317000	3.717900000
N	-4.469867000	-0.249736000	3.855499000	C	-4.244317000	-1.125766000	2.796851000
N	-3.895420000	-2.312902000	3.397352000	C	-3.902985000	-2.197636000	4.799190000
N	0.215760000	3.737992000	1.077403000	C	-4.267588000	-0.901352000	5.089827000
N	-1.583912000	-3.444031000	1.081360000	C	-1.528792000	4.662770000	2.613443000
N	-2.207815000	-3.710549000	-3.814640000	C	-0.136900000	4.150343000	2.339630000
N	-3.895883000	-2.379235000	-3.398935000	C	-3.542207000	-3.550671000	2.639270000
N	-4.157003000	0.200854000	-1.062322000	C	-2.067532000	-3.675652000	2.347170000
N	-3.797187000	1.554866000	-1.063704000	C	-2.892838000	-3.083983000	-2.775286000
N	-2.333327000	3.721709000	-3.399945000	C	-2.790131000	-3.386447000	-5.058442000
N	-0.241972000	4.223394000	-3.817083000	C	-3.849028000	-2.545884000	-4.795097000
C	4.244632000	1.126202000	2.796739000	C	-4.905702000	-1.565866000	-2.660739000
C	3.903949000	2.198329000	4.799054000	C	-4.426436000	-0.169955000	-2.357401000
C	4.268560000	0.902061000	5.089740000	C	-4.240863000	0.945760000	-3.204491000
C	4.936479000	-1.147951000	3.717857000	C	-3.848232000	2.008461000	-2.357880000
C	3.231463000	-2.799623000	2.783407000	C	-3.601981000	3.464404000	-2.657812000
C	2.482868000	-3.653070000	4.780972000	C	-1.125915000	3.938864000	-2.777180000
C	3.408722000	-2.677602000	5.078387000	C	-0.907583000	4.172710000	-5.060731000
C	3.542579000	3.551022000	2.638961000	C	-2.221191000	3.854307000	-4.796500000
C	2.067869000	3.675767000	2.346915000	C	1.006969000	4.116668000	3.171116000
C	1.529063000	-4.662787000	2.614004000	C	-1.006684000	-4.116596000	3.171441000
C	0.137161000	-4.150517000	2.339963000	C	-1.141026000	-4.721080000	-3.636588000
C	1.126126000	-3.939540000	-2.776848000	C	1.141225000	4.720560000	-3.636950000
C	0.907687000	-4.172870000	-5.060430000	H	3.691417000	3.032162000	5.456431000
C	2.221263000	-3.854317000	-4.796210000	H	4.432242000	0.418576000	6.044877000

H	5.678115000	-1.339290000	4.505117000	H	-1.067730000	-4.413459000	4.213427000
H	5.402518000	-1.262568000	2.733307000	H	-1.226541000	-5.133514000	-2.625566000
H	1.926354000	-4.314682000	5.433009000	H	-1.308370000	-5.517154000	-4.374792000
H	3.798481000	-2.351314000	6.034772000	H	1.226705000	5.133112000	-2.625975000
H	4.103631000	3.528037000	1.693771000	H	1.308500000	5.516588000	-4.375217000
H	3.888795000	4.409028000	3.232823000	H	3.066860000	-3.751155000	-5.464933000
H	1.482103000	-5.596397000	3.193042000	C	0.613097000	0.053981000	-0.411331000
H	2.037328000	-4.866790000	1.660762000	C	-0.613616000	-0.049644000	-0.411116000
H	0.418655000	-4.397997000	-6.000229000	H	1.682309000	0.143510000	-0.403698000
H	4.422582000	-3.876841000	-3.262762000	H	-1.682848000	-0.139570000	-0.404217000
H	3.546447000	-4.025431000	-1.713424000	<u>C₂H₄@PPX</u>			
H	4.402899000	-0.988229000	-4.276128000	Au	-3.963433000	-1.592971000	0.832984000
H	5.127013000	2.088313000	-1.719107000	Au	-3.894689000	1.557725000	0.843091000
H	5.818844000	1.540302000	-3.273042000	Au	-1.577809000	3.703345000	-0.821981000
H	2.439871000	3.795703000	-5.997917000	Au	-1.583449000	-3.642418000	-0.836816000
H	4.572469000	2.095416000	-5.464172000	Au	3.960021000	-1.599937000	0.832823000
H	-1.926056000	4.315114000	5.432454000	Au	3.898872000	1.550859000	0.842768000
H	-3.798384000	2.352004000	6.034534000	Au	1.584398000	3.699098000	-0.822273000
H	-5.677984000	1.339568000	4.505275000	Au	1.576168000	-3.645333000	-0.836895000
H	-5.402703000	1.262754000	2.733429000	N	-3.214869000	-3.131693000	3.378765000
H	-3.690230000	-3.031380000	5.456610000	N	-4.245633000	-1.256023000	3.845052000
H	-4.431063000	-0.417768000	6.044947000	N	-4.232971000	1.231737000	3.852508000
H	-2.036929000	4.866610000	1.660095000	N	-3.198382000	3.108347000	3.398993000
H	-1.481788000	5.596519000	3.192261000	N	-0.704515000	-3.738312000	1.068131000
H	-3.888416000	-4.408569000	3.233295000	N	-0.696258000	3.802679000	1.077629000
H	-4.103317000	-3.527849000	1.694108000	N	-1.246291000	4.114560000	-3.820079000
H	-2.439858000	-3.796735000	-5.997607000	N	-3.169699000	3.158714000	-3.389005000
H	-4.572326000	-2.096199000	-5.464059000	N	-4.039130000	0.690971000	-1.058756000
H	-5.818589000	-1.540909000	-3.272973000	N	-4.055078000	-0.707971000	-1.064614000
H	-5.126592000	-2.088514000	-1.718971000	N	-3.188923000	-3.151323000	-3.407510000
H	-4.401617000	0.987550000	-4.276542000	N	-1.255928000	-4.091541000	-3.829080000
H	-3.546191000	4.025117000	-1.713735000	N	3.208740000	-3.137116000	3.378721000
H	-4.422358000	3.876676000	-3.263070000	N	4.243383000	-1.263545000	3.844895000
H	-0.418550000	4.397962000	-6.000497000	N	4.235981000	1.224220000	3.852220000
H	-3.066844000	3.751353000	-5.465183000	N	3.204926000	3.102715000	3.398495000
H	1.067980000	4.413716000	4.213051000	N	0.697198000	-3.739473000	1.068111000

N	0.703403000	3.801151000	1.077484000	C	2.593288000	-4.263453000	2.615649000
N	1.254000000	4.112127000	-3.820220000	C	1.123885000	-4.071589000	2.331834000
N	3.175701000	3.152747000	-3.389386000	C	2.601548000	4.240365000	2.643041000
N	4.041038000	0.683625000	-1.059053000	C	1.131465000	4.068331000	2.355029000
N	4.053853000	-0.715340000	-1.064802000	C	2.055887000	3.660805000	-2.773052000
N	3.182094000	-3.157064000	-3.407725000	C	1.882781000	3.878390000	-5.061548000
N	1.247346000	-4.093713000	-3.829192000	C	3.089217000	3.272156000	-4.788501000
C	-3.820519000	-2.049557000	2.782093000	C	4.340090000	2.590988000	-2.642544000
C	-3.257129000	-3.031953000	4.781370000	C	4.215127000	1.117616000	-2.350450000
C	-3.908205000	-1.854610000	5.076974000	C	4.335739000	-0.005130000	-3.201472000
C	-5.031071000	-0.007976000	3.712732000	C	4.229832000	-1.136100000	-2.359253000
C	-3.777628000	2.016343000	2.794461000	C	4.354997000	-2.606048000	-2.666218000
C	-3.281648000	3.021992000	4.800632000	C	2.052435000	-3.637156000	-2.786822000
C	-3.934857000	1.844040000	5.088190000	C	1.882350000	-3.887525000	-5.072311000
C	-2.601432000	-4.259120000	2.615693000	C	3.096973000	-3.295380000	-4.805335000
C	-1.131715000	-4.069747000	2.331850000	C	-0.004079000	-4.281554000	3.158622000
C	-2.593209000	4.245159000	2.643666000	C	0.004250000	4.240401000	3.191596000
C	-1.123502000	4.070622000	2.355294000	C	0.004603000	4.890044000	-3.656101000
C	-2.049174000	3.665361000	-2.772788000	C	-0.004946000	-4.864495000	-3.655794000
C	-1.875194000	3.881027000	-5.061387000	H	-2.865630000	-3.800943000	5.435598000
C	-3.082706000	3.277010000	-4.788185000	H	-4.183313000	-1.428609000	6.033956000
C	-4.334998000	2.599150000	-2.641956000	H	-5.799294000	-0.005349000	4.497698000
C	-4.212863000	1.125483000	-2.350028000	H	-5.508310000	-0.002955000	2.726933000
C	-4.336276000	0.003080000	-3.201109000	H	-2.913732000	3.799460000	5.458551000
C	-4.232484000	-1.128210000	-2.359058000	H	-4.236894000	1.426009000	6.040582000
C	-4.360761000	-2.597860000	-2.666113000	H	-3.149321000	-4.346010000	1.666658000
C	-2.060076000	-3.633406000	-2.786666000	H	-2.761450000	-5.176537000	3.200122000
C	-1.890726000	-3.884442000	-5.072142000	H	-2.761609000	5.156401000	3.235552000
C	-3.104210000	-3.289991000	-4.805112000	H	-3.142678000	4.335362000	1.695855000
C	3.816419000	-2.056153000	2.781970000	H	-1.444913000	4.188203000	-6.006697000
C	3.251466000	-3.037522000	4.781322000	H	-5.234125000	2.801020000	-3.242016000
C	3.904980000	-1.861516000	5.076855000	H	-4.412537000	3.152241000	-1.694941000
C	5.031482000	-0.017154000	3.712542000	H	-4.512737000	0.008479000	-4.271577000
C	3.782417000	2.009730000	2.794100000	H	-4.448289000	-3.160226000	-1.725334000
C	3.287719000	3.016199000	4.800151000	H	-5.254409000	-2.791278000	-3.276868000
C	3.938583000	1.836982000	5.087851000	H	-1.459130000	-4.201086000	-6.013715000

H	-3.904952000	-2.997098000	-5.472877000	Au	-1.764712000	3.643052000	-0.825025000
H	2.858549000	-3.805755000	5.435588000	Au	-1.414701000	-3.743695000	-0.826331000
H	4.181127000	-1.436107000	6.033802000	Au	4.021653000	-1.408123000	0.831110000
H	5.799673000	-0.016137000	4.497543000	Au	3.837365000	1.730445000	0.832870000
H	5.508764000	-0.013189000	2.726753000	Au	1.388674000	3.714716000	-0.833261000
H	2.921077000	3.794329000	5.457992000	Au	1.736166000	-3.576902000	-0.832576000
H	4.239570000	1.418349000	6.040311000	N	-3.062138000	-3.264133000	3.392100000
H	3.141070000	-4.351257000	1.666632000	N	-4.179176000	-1.436005000	3.847720000
H	2.751748000	-5.181152000	3.200066000	N	-4.289633000	1.050216000	3.850199000
H	2.771607000	5.151470000	3.234661000	N	-3.349228000	2.976029000	3.398850000
H	3.150926000	4.329439000	1.695078000	N	-0.530621000	-3.783086000	1.076743000
H	1.453210000	4.186931000	-6.006740000	N	-0.885748000	3.750482000	1.076621000
H	3.884383000	2.959212000	-5.453810000	N	-1.448489000	4.065988000	-3.821738000
H	5.239452000	2.791082000	-3.242845000	N	-3.326224000	3.022476000	-3.392292000
H	4.418967000	3.143938000	-1.695568000	N	-4.050682000	0.517378000	-1.061195000
H	4.511777000	-0.000216000	-4.272010000	N	-3.987750000	-0.879223000	-1.062506000
H	4.441131000	-3.168616000	-1.725421000	N	-3.032006000	-3.303247000	-3.396278000
H	5.248327000	-2.801407000	-3.276819000	N	-1.067274000	-4.174877000	-3.819797000
H	1.450066000	-4.203226000	-6.013882000	N	3.354456000	-2.973272000	3.382458000
H	3.898178000	-3.003879000	-5.473151000	N	4.305651000	-1.054767000	3.842165000
H	-0.004326000	-4.586402000	4.200086000	N	4.187963000	1.428839000	3.842711000
H	0.004623000	4.495142000	4.246369000	N	3.060399000	3.249391000	3.382972000
H	0.005068000	5.331508000	-2.653824000	N	0.868670000	-3.716048000	1.073609000
H	0.005365000	5.688247000	-4.410791000	N	0.513806000	3.797870000	1.072094000
H	-0.005262000	-5.293586000	-2.648188000	N	1.049671000	4.165794000	-3.826757000
H	-0.005690000	-5.672359000	-4.400182000	N	3.011629000	3.288604000	-3.402420000
H	-3.878253000	2.964957000	-5.453455000	N	4.010205000	0.865835000	-1.067270000
C	0.677523000	-0.034542000	-0.205558000	N	4.083701000	-0.530339000	-1.070015000
C	-0.676613000	-0.031348000	-0.208964000	N	3.315094000	-3.023570000	-3.406947000
H	1.242576000	-0.851809000	0.251142000	N	1.431380000	-4.061525000	-3.823008000
H	-1.247800000	-0.845944000	0.244862000	C	-3.698967000	-2.203686000	2.788805000
H	1.264532000	0.772239000	-0.654590000	C	-3.137232000	-3.175803000	4.794156000
H	-1.257520000	0.778231000	-0.660900000	C	-3.842497000	-2.028409000	5.083060000
<u>C₂H₆@PPX</u>				C	-5.023454000	-0.227952000	3.706713000
Au	-3.833376000	-1.747142000	0.838449000	C	-3.870466000	1.855559000	2.793013000
Au	-3.954784000	1.388857000	0.842248000	C	-3.433659000	2.886811000	4.800381000

C	-4.027524000	1.677398000	5.086442000	C	2.058912000	-3.836604000	-5.066707000
C	-2.399003000	-4.366140000	2.633937000	C	3.241220000	-3.180845000	-4.803023000
C	-0.940138000	-4.112473000	2.346154000	C	0.197499000	-4.256639000	3.174023000
C	-2.794248000	4.138444000	2.643644000	C	-0.196058000	4.247370000	3.181157000
C	-1.319186000	4.022349000	2.351652000	C	-0.230300000	4.891021000	-3.655826000
C	-2.234151000	3.586909000	-2.775134000	C	0.216838000	-4.890790000	-3.646687000
C	-2.059993000	3.795324000	-5.064102000	H	-2.727674000	-3.932402000	5.451815000
C	-3.238491000	3.135930000	-4.791823000	H	-4.154910000	-1.620541000	6.036534000
C	-4.461604000	2.401368000	-2.647229000	H	-5.797370000	-0.262479000	4.485314000
C	-4.257571000	0.937460000	-2.351765000	H	-5.492251000	-0.248002000	2.717042000
C	-4.326408000	-0.193189000	-3.198768000	H	-3.107987000	3.682274000	5.459096000
C	-4.154637000	-1.314396000	-2.353992000	H	-4.311529000	1.245213000	6.038063000
C	-4.221370000	-2.790348000	-2.652651000	H	-2.944134000	-4.482218000	1.686326000
C	-1.889879000	-3.754085000	-2.776386000	H	-2.517654000	-5.286747000	3.223251000
C	-1.705379000	-3.979838000	-5.063012000	H	-2.998036000	5.041466000	3.236850000
C	-2.939147000	-3.428873000	-4.794570000	H	-3.349243000	4.206463000	1.697058000
C	3.907019000	-1.865310000	2.781642000	H	-1.640553000	4.116533000	-6.009609000
C	3.402943000	-2.872546000	4.784865000	H	-5.368665000	2.552064000	-3.250326000
C	4.003775000	-1.667866000	5.076320000	H	-4.572073000	2.950482000	-1.701196000
C	5.038526000	0.224301000	3.705810000	H	-4.514192000	-0.200911000	-4.267353000
C	3.698669000	2.188568000	2.782002000	H	-4.281734000	-3.350395000	-1.708319000
C	3.142539000	3.168873000	4.785100000	H	-5.109321000	-3.023347000	-3.257867000
C	3.854188000	2.026200000	5.076582000	H	-1.261315000	-4.274615000	-6.005866000
C	2.790374000	-4.128175000	2.623116000	H	-3.747625000	-3.158323000	-5.462428000
C	1.313155000	-4.007001000	2.341411000	H	3.050894000	-3.658407000	5.441461000
C	2.397021000	4.349048000	2.622367000	H	4.267779000	-1.230690000	6.031389000
C	0.934921000	4.104422000	2.343674000	H	5.806249000	0.261154000	4.490380000
C	1.864212000	3.727364000	-2.783546000	H	5.514351000	0.246898000	2.719513000
C	1.697425000	3.990120000	-5.068131000	H	2.732948000	3.927206000	5.440711000
C	2.929424000	3.435834000	-4.799231000	H	4.173227000	1.624786000	6.030609000
C	4.201327000	2.780174000	-2.657487000	H	3.339328000	-4.192746000	1.672899000
C	4.143508000	1.303801000	-2.361631000	H	2.993069000	-5.036270000	3.208955000
C	4.300086000	0.185204000	-3.212542000	H	2.523961000	5.272589000	3.205484000
C	4.258785000	-0.946767000	-2.365892000	H	2.936574000	4.457448000	1.670725000
C	4.458213000	-2.408912000	-2.668779000	H	1.260295000	4.299936000	-6.009438000
C	2.209617000	-3.553954000	-2.783394000	H	3.743242000	3.176423000	-5.465034000

H	5.089199000	3.019407000	-3.260587000	N	-0.085967000	3.622041000	1.084080000
H	4.257990000	3.338620000	-1.711960000	N	-0.632896000	4.042872000	-3.789735000
H	4.460879000	0.195256000	-4.285441000	N	-2.706103000	3.463087000	-3.369553000
H	4.575959000	-2.962084000	-1.725911000	N	-4.246921000	1.279887000	-1.032522000
H	5.359512000	-2.559983000	-3.280340000	N	-4.494900000	-0.098003000	-1.041448000
H	1.646110000	-4.184113000	-6.005854000	N	-3.731975000	-2.609879000	-3.403554000
H	4.028613000	-2.855978000	-5.471877000	N	-1.881431000	-3.716400000	-3.800888000
H	0.213239000	-4.545157000	4.219996000	N	2.682985000	-3.423053000	3.365182000
H	-0.202524000	4.519194000	4.231661000	N	4.073486000	-1.803183000	3.857956000
H	-0.245929000	5.326196000	-2.650885000	N	4.524440000	0.629466000	3.857007000
H	-0.262876000	5.692865000	-4.405911000	N	3.749967000	2.616232000	3.360277000
H	0.236980000	-5.317469000	-2.638212000	N	0.084317000	-3.615096000	1.079538000
H	0.253484000	-5.698754000	-4.390006000	N	1.305994000	3.455626000	1.075123000
H	-4.015385000	2.782181000	-5.458243000	N	1.865799000	3.722996000	-3.807426000
C	-0.769508000	-0.071217000	-0.212815000	N	3.712914000	2.610235000	-3.412917000
C	0.752251000	0.180274000	-0.070605000	N	4.496232000	0.091098000	-1.050784000
H	-1.297474000	0.836401000	-0.545985000	N	4.257762000	-1.290053000	-1.044292000
H	0.955084000	0.964596000	0.679269000	N	2.695637000	-3.464488000	-3.382154000
H	-1.216004000	-0.379876000	0.748768000	N	0.618478000	-4.036870000	-3.792287000
H	1.204281000	0.516480000	-1.019946000	C	-4.255310000	-1.478016000	2.794070000
H	-0.983833000	-0.868239000	-0.945426000	C	-3.682545000	-2.498607000	4.772197000
H	1.275614000	-0.739277000	0.241727000	C	-4.169676000	-1.249776000	5.086887000
<u>Allene</u>				C	-5.081314000	0.733976000	3.766353000
Au	-4.473717000	-1.014892000	0.850585000	C	-3.510905000	2.500360000	2.792665000
Au	-3.839073000	2.106476000	0.850345000	C	-2.700228000	3.327824000	4.778447000
Au	-1.017614000	3.631017000	-0.800130000	C	-3.573061000	2.309752000	5.090475000
Au	-2.198064000	-3.247688000	-0.817472000	C	-3.265009000	-3.802732000	2.600045000
Au	3.873493000	-2.126628000	0.841781000	C	-1.779576000	-3.779950000	2.326261000
Au	4.473769000	1.010575000	0.838136000	C	-1.889131000	4.440957000	2.610629000
Au	2.180928000	3.235107000	-0.824243000	C	-0.457760000	4.045450000	2.337989000
Au	1.015448000	-3.609747000	-0.806069000	C	-1.506771000	3.727929000	-2.747354000
N	-3.740596000	-2.616581000	3.371835000	C	-1.297862000	3.962537000	-5.032412000
N	-4.511075000	-0.628154000	3.868128000	C	-2.598102000	3.594990000	-4.766839000
N	-4.063357000	1.805521000	3.867908000	C	-3.972836000	3.173063000	-2.633036000
N	-2.676434000	3.428165000	3.375462000	C	-4.176639000	1.709970000	-2.334661000
N	-1.308477000	-3.453348000	1.076187000	C	-4.380413000	0.608122000	-3.196112000

C	-4.570018000	-0.507727000	-2.348706000	H	-3.906123000	1.944712000	6.054162000
C	-4.857663000	-1.950059000	-2.677733000	H	-3.817298000	-3.816327000	1.649669000
C	-2.662091000	-3.195377000	-2.768275000	H	-3.532661000	-4.700492000	3.175652000
C	-2.475391000	-3.445253000	-5.052671000	H	-1.917332000	5.377027000	3.187219000
C	-3.634819000	-2.745566000	-4.801031000	H	-2.412233000	4.602835000	1.657377000
C	3.530965000	-2.506857000	2.783794000	H	-0.818999000	4.203614000	-5.973478000
C	2.690245000	-3.308050000	4.767276000	H	-4.798468000	3.564769000	-3.245327000
C	3.565345000	-2.291954000	5.079540000	H	-3.939743000	3.736013000	-1.689266000
C	5.093711000	-0.733160000	3.756706000	H	-4.417306000	0.620613000	-4.280168000
C	4.262440000	1.476753000	2.781984000	H	-5.026975000	-2.511386000	-1.747515000
C	3.699960000	2.501798000	4.761191000	H	-5.752230000	-2.040216000	-3.311256000
C	4.189491000	1.254017000	5.076120000	H	-2.059698000	-3.793391000	-5.990250000
C	1.894422000	-4.435508000	2.600922000	H	-4.394960000	-2.378232000	-5.479495000
C	0.461985000	-4.040589000	2.331328000	H	2.118791000	-3.964505000	5.411346000
C	3.270013000	3.800451000	2.588551000	H	3.888387000	-1.918600000	6.043412000
C	1.782942000	3.778834000	2.323891000	H	5.809762000	-0.866594000	4.578858000
C	2.641223000	3.191143000	-2.776512000	H	5.609605000	-0.829423000	2.795522000
C	2.464577000	3.462408000	-5.059425000	H	3.365347000	3.307649000	5.402325000
C	3.622143000	2.759077000	-4.809466000	H	4.358806000	0.791212000	6.040389000
C	4.836007000	1.948304000	-2.686596000	H	2.416472000	-4.597747000	1.647111000
C	4.547290000	0.506271000	-2.357406000	H	1.922830000	-5.371691000	3.177387000
C	4.346772000	-0.605797000	-3.206996000	H	3.542552000	4.699710000	3.159531000
C	4.164547000	-1.712399000	-2.347931000	H	3.815379000	3.810797000	1.634016000
C	3.964634000	-3.174772000	-2.650348000	H	2.053126000	3.820234000	-5.995262000
C	1.495948000	-3.713291000	-2.755034000	H	4.384611000	2.396689000	-5.487982000
C	1.282348000	-3.974973000	-5.036722000	H	5.731316000	2.036280000	-3.319528000
C	2.585044000	-3.612053000	-4.777499000	H	5.006816000	2.509313000	-1.756369000
C	-0.688818000	-4.149620000	3.147496000	H	4.364344000	-0.612584000	-4.291508000
C	0.696276000	4.149482000	3.150346000	H	3.937823000	-3.740809000	-1.708146000
C	0.715315000	4.636392000	-3.613138000	H	4.788434000	-3.562470000	-3.267737000
C	-0.729565000	-4.628952000	-3.609193000	H	0.800890000	-4.225020000	-5.974090000
H	-3.344088000	-3.302738000	5.413443000	H	3.426351000	-3.487374000	-5.448073000
H	-4.332431000	-0.784177000	6.050939000	H	-0.731179000	-4.492320000	4.176365000
H	-5.798597000	0.867454000	4.587426000	H	0.743210000	4.489355000	4.179925000
H	-5.596211000	0.828730000	2.804467000	H	0.774268000	5.046307000	-2.599347000
H	-2.140969000	3.994695000	5.422531000	H	0.813511000	5.451010000	-4.343852000

H	-0.784958000	-5.037498000	-2.594781000	N	-4.333046000	-0.696944000	-1.020749000
H	-0.830265000	-5.445042000	-4.337914000	N	-4.305586000	-1.235087000	3.895459000
H	-3.439729000	3.458361000	-5.434647000	N	-3.215051000	-3.065014000	3.388821000
C	1.292420000	-0.097677000	-0.430548000	N	-0.689385000	-3.521150000	1.085463000
C	-0.011443000	0.040141000	-0.612056000	N	0.713079000	-3.524171000	1.078685000
H	1.820786000	0.494229000	0.319172000	N	3.267308000	-3.072352000	3.354363000
C	-1.322412000	0.160773000	-0.747225000	N	4.364253000	-1.240481000	3.842848000
H	-1.995784000	-0.428556000	-0.125180000	C	2.053682000	3.492575000	-2.783483000
H	-1.777634000	0.853446000	-1.455410000	C	3.113212000	3.278104000	-4.811736000
H	1.878568000	-0.808389000	-1.012703000	C	1.872173000	3.822531000	-5.057824000
<u>C₃H₄@PPX</u>				C	-0.028713000	4.711131000	-3.603013000
Au	1.584100000	3.426824000	-0.832635000	C	-2.098037000	3.495956000	-2.754084000
Au	-1.585859000	3.408959000	-0.814908000	C	-3.189040000	3.284124000	-4.767227000
Au	-4.122585000	1.568474000	0.873297000	C	-1.951900000	3.827983000	-5.032060000
Au	4.138277000	1.570747000	0.823123000	C	4.410846000	2.595226000	-2.693648000
Au	1.579706000	-3.428192000	-0.832356000	C	4.345145000	1.123615000	-2.381355000
Au	-1.590797000	-3.408205000	-0.814716000	C	-4.455340000	2.602005000	-2.630343000
Au	-4.124794000	-1.564051000	0.873394000	C	-4.391208000	1.129408000	-2.322488000
Au	4.136172000	-1.575089000	0.823205000	C	-3.880805000	2.011320000	2.815464000
N	3.205324000	3.092769000	-3.419867000	C	-3.903269000	1.827754000	5.113487000
N	1.228049000	3.953396000	-3.808779000	C	-3.213442000	2.975649000	4.792244000
N	-1.288453000	3.956648000	-3.792544000	C	-2.570351000	4.164024000	2.603697000
N	-3.259570000	3.096453000	-3.373738000	C	-1.104391000	3.936986000	2.326260000
N	4.285352000	0.698127000	-1.078173000	C	0.027510000	4.201030000	3.133055000
N	-4.331888000	0.701478000	-1.020641000	C	1.151600000	3.940279000	2.316716000
N	-4.303886000	1.240068000	3.895347000	C	2.620273000	4.168005000	2.579434000
N	-3.210883000	3.068485000	3.388557000	C	3.931623000	2.012281000	2.770462000
N	-0.684494000	3.521320000	1.085388000	C	3.983161000	1.823065000	5.067236000
N	0.717969000	3.523406000	1.078592000	C	3.292343000	2.973640000	4.757340000
N	3.271585000	3.069775000	3.354093000	C	2.049446000	-3.494728000	-2.783149000
N	4.366142000	1.236522000	3.842763000	C	3.109586000	-3.282391000	-4.811326000
N	3.201653000	-3.096550000	-3.419514000	C	1.867940000	-3.825414000	-5.057406000
N	1.223406000	-3.954952000	-3.808424000	C	-0.034363000	-4.711031000	-3.602738000
N	-1.293135000	-3.954922000	-3.792412000	C	-2.102688000	-3.494019000	-2.754021000
N	-3.263420000	-3.092612000	-3.373960000	C	-3.192392000	-3.279315000	-4.767550000
N	4.284459000	-0.702818000	-1.078132000	C	-1.955784000	-3.824510000	-5.032156000

C	4.407706000	-2.600233000	-2.693321000	H	2.859404000	3.727667000	5.402695000
C	4.343751000	-1.128492000	-2.381260000	H	3.923374000	-3.054038000	-5.488556000
C	-4.458869000	-2.596998000	-2.630818000	H	1.420800000	-4.154225000	-5.987488000
C	-4.393052000	-1.124504000	-2.322720000	H	-0.038105000	-5.544861000	-4.318141000
C	-3.883435000	-2.006909000	2.815641000	H	-0.028430000	-5.106529000	-2.581469000
C	-3.905824000	-1.823242000	5.113653000	H	-4.016551000	-3.051297000	-5.432278000
C	-3.217552000	-2.972100000	4.792492000	H	-1.523596000	-4.155023000	-5.968689000
C	-2.575768000	-4.161349000	2.604081000	H	4.484480000	-3.168384000	-1.754995000
C	-1.109602000	-3.935730000	2.326568000	H	5.282619000	-2.831666000	-3.318061000
C	0.022082000	-4.200149000	3.133538000	H	-5.343032000	-2.831553000	-3.241262000
C	1.146370000	-3.940717000	2.317056000	H	-4.519843000	-3.162390000	-1.689674000
C	2.614807000	-4.169925000	2.579783000	H	-4.169510000	-1.412428000	6.080425000
C	3.929060000	-2.015992000	2.770636000	H	-2.776119000	-3.727347000	5.430593000
C	3.979972000	-1.826082000	5.067363000	H	-2.713745000	-5.094670000	3.168656000
C	3.287633000	-2.975771000	4.757578000	H	-3.121268000	-4.241246000	1.653031000
C	4.386018000	-0.002499000	-3.234500000	H	0.025757000	-4.572860000	4.152839000
C	-4.430800000	0.002565000	-3.177025000	H	3.150686000	-4.255175000	1.623717000
C	-5.110922000	0.003037000	3.794815000	H	2.755967000	-5.101221000	3.146684000
C	5.169248000	-0.002588000	3.729154000	H	4.255541000	-1.413109000	6.029915000
H	3.926603000	3.048531000	-5.489030000	H	2.853428000	-3.729001000	5.403012000
H	1.425286000	4.151514000	-5.987968000	H	4.463723000	-0.002592000	-4.316434000
H	-0.031443000	5.544934000	-4.318450000	H	-4.513145000	0.002736000	-4.258723000
H	-0.022144000	5.106660000	-2.581761000	H	-5.630675000	0.003362000	2.830615000
H	-4.013802000	3.057582000	-5.431710000	H	-5.841928000	0.003578000	4.614380000
H	-1.519795000	4.158717000	-5.968555000	H	5.673520000	-0.003024000	2.756747000
H	4.488294000	3.163466000	-1.755432000	H	5.913351000	-0.003116000	4.536832000
H	5.286002000	2.825521000	-3.318468000	H	-2.770998000	3.730355000	5.430282000
H	-5.339413000	2.837623000	-3.240508000	C	-1.164944000	-0.001868000	-1.330983000
H	-4.515464000	3.167321000	-1.689095000	C	-0.204151000	-0.000754000	-0.561439000
H	-4.167479000	1.417377000	6.080303000	H	-1.989994000	-0.004196000	-2.010446000
H	-2.707372000	5.097565000	3.168143000	C	0.974373000	-0.000322000	0.318815000
H	-3.115726000	4.244371000	1.652608000	H	1.890802000	-0.000254000	-0.287861000
H	0.031487000	4.574177000	4.152196000	H	0.995933000	0.899550000	0.955062000
H	3.156256000	4.252636000	1.623369000	H	0.996013000	-0.899954000	0.955460000
H	2.762379000	5.099168000	3.146304000	<u>C₃H₆@PPX</u>			
H	4.258496000	1.409990000	6.029812000	Au	1.427723000	3.525871000	-0.831206000

Au	-1.699116000	3.405184000	-0.829717000	C	-3.275656000	3.226732000	-4.788438000
Au	-4.095315000	1.417078000	0.847909000	C	-2.071935000	3.844856000	-5.045514000
Au	3.949804000	1.678382000	0.824175000	C	4.267692000	2.738882000	-2.675949000
Au	1.704192000	-3.417472000	-0.835214000	C	4.214301000	1.263923000	-2.377528000
Au	-1.430256000	-3.489021000	-0.825329000	C	-4.495893000	2.441333000	-2.658906000
Au	-3.989807000	-1.698007000	0.848437000	C	-4.338054000	0.975185000	-2.354228000
Au	4.108924000	-1.436443000	0.819510000	C	-3.943064000	1.878755000	2.795230000
N	3.068161000	3.238025000	-3.409818000	C	-4.037971000	1.712474000	5.092354000
N	1.087905000	4.084628000	-3.807060000	C	-3.398150000	2.892761000	4.784029000
N	-1.418188000	3.996745000	-3.803634000	C	-2.743459000	4.095118000	2.604163000
N	-3.335373000	3.018925000	-3.397796000	C	-1.271096000	3.916462000	2.330182000
N	4.098284000	0.827134000	-1.081238000	C	-0.150603000	4.198117000	3.146455000
N	-4.217508000	0.552497000	-1.054853000	C	0.983188000	3.988629000	2.328388000
N	-4.364304000	1.095110000	3.866641000	C	2.442369000	4.259941000	2.599088000
N	-3.351091000	2.974254000	3.380535000	C	3.797998000	2.132246000	2.773078000
N	-0.833823000	3.538050000	1.083583000	C	3.924460000	1.966716000	5.068366000
N	0.565706000	3.583592000	1.081973000	C	3.193945000	3.095643000	4.769430000
N	3.129113000	3.177967000	3.366512000	C	2.184497000	-3.487870000	-2.783287000
N	4.286703000	1.379340000	3.837864000	C	3.240475000	-3.241746000	-4.810085000
N	3.315147000	-3.033463000	-3.420473000	C	2.031814000	-3.855730000	-5.054214000
N	1.390236000	-4.004230000	-3.805999000	C	0.160621000	-4.801506000	-3.596160000
N	-1.117569000	-4.082340000	-3.796131000	C	-1.931254000	-3.610695000	-2.766418000
N	-3.099014000	-3.241198000	-3.392140000	C	-3.028656000	-3.457450000	-4.780953000
N	4.162403000	-0.570504000	-1.085556000	C	-1.784391000	-3.989496000	-5.036756000
N	-4.166731000	-0.844813000	-1.054883000	C	4.481832000	-2.450624000	-2.694623000
N	-4.263318000	-1.380707000	3.867094000	C	4.313609000	-0.986929000	-2.384084000
N	-3.104594000	-3.174308000	3.381687000	C	-4.300405000	-2.750160000	-2.655693000
N	-0.551254000	-3.555077000	1.084977000	C	-4.254396000	-1.276019000	-2.354093000
N	0.849497000	-3.522814000	1.079638000	C	-3.791475000	-2.135752000	2.796521000
N	3.380576000	-2.980702000	3.360558000	C	-3.873868000	-1.959965000	5.092902000
N	4.392309000	-1.097567000	3.835524000	C	-3.142615000	-3.086085000	4.785051000
C	1.908132000	3.622297000	-2.778916000	C	-2.419525000	-4.249342000	2.605327000
C	2.987398000	3.438001000	-4.800306000	C	-0.962753000	-3.971496000	2.329165000
C	1.743572000	3.973621000	-5.051863000	C	0.174209000	-4.196792000	3.139389000
C	-0.191836000	4.801234000	-3.605521000	C	1.292144000	-3.915619000	2.321033000
C	-2.200078000	3.478487000	-2.772018000	C	2.764847000	-4.102749000	2.591211000

C	3.978180000	-1.891331000	2.769389000	H	-2.691737000	-3.828586000	5.431535000
C	4.058262000	-1.703447000	5.064883000	H	-2.523307000	-5.183305000	3.176079000
C	3.419187000	-2.885949000	4.763650000	H	-2.958788000	-4.357423000	1.653424000
C	4.349554000	0.144866000	-3.230518000	H	0.187120000	-4.560119000	4.162031000
C	-4.364485000	-0.153125000	-3.206006000	H	3.306842000	-4.180944000	1.638060000
C	-5.114524000	-0.175206000	3.747960000	H	2.929218000	-5.024866000	3.166668000
C	5.138061000	0.174577000	3.708460000	H	4.328645000	-1.278515000	6.023693000
H	3.808986000	3.223484000	-5.472578000	H	3.033923000	-3.661177000	5.414145000
H	1.301488000	4.308623000	-5.982164000	H	4.489932000	0.154082000	-4.306196000
H	-0.221783000	5.635837000	-4.319223000	H	-4.484188000	-0.157702000	-4.284272000
H	-0.204140000	5.192630000	-2.582557000	H	-5.610950000	-0.195903000	2.771766000
H	-4.084895000	2.959096000	-5.456657000	H	-5.864544000	-0.205406000	4.549583000
H	-1.658750000	4.211001000	-5.977365000	H	5.623012000	0.195866000	2.726425000
H	4.330727000	3.298307000	-1.731447000	H	5.897133000	0.206836000	4.501511000
H	5.148645000	2.980042000	-3.288113000	H	-3.017317000	3.674217000	5.429698000
H	-5.392678000	2.618731000	-3.270096000	C	-0.798545000	0.058715000	-0.961867000
H	-4.595359000	2.998604000	-1.716226000	C	0.430201000	0.165630000	-0.394110000
H	-4.313568000	1.295959000	6.053405000	H	-0.959504000	0.182015000	-2.036678000
H	-2.913822000	5.019726000	3.174036000	H	-1.680241000	-0.147354000	-0.349765000
H	-3.286679000	4.163354000	1.650920000	C	0.678805000	0.019067000	1.093004000
H	-0.160895000	4.550755000	4.172831000	H	1.309557000	0.378892000	-1.014425000
H	2.977647000	4.371347000	1.645344000	H	1.169745000	0.925614000	1.489128000
H	2.552974000	5.189699000	3.175237000	H	-0.268348000	-0.143500000	1.634337000
H	4.239038000	1.569889000	6.025769000	H	1.345320000	-0.838522000	1.289258000
H	2.760203000	3.843934000	5.420954000	<u>C₃H₈@PPX</u>			
H	4.043425000	-2.976800000	-5.486890000	Au	-1.848272000	-3.448099000	-0.816695000
H	1.607387000	-4.220334000	-5.981597000	Au	1.300993000	-3.624855000	-0.837572000
H	0.183971000	-5.641095000	-4.304258000	Au	3.913920000	-1.832995000	0.823294000
H	0.176237000	-5.186726000	-2.571033000	Au	-4.116214000	-1.296170000	0.865442000
H	-3.857301000	-3.255640000	-5.448514000	Au	-1.299902000	3.623615000	-0.828951000
H	-1.348760000	-4.333713000	-5.966734000	Au	1.848501000	3.464006000	-0.837394000
H	4.598551000	-3.010547000	-1.755493000	Au	4.130482000	1.298423000	0.832725000
H	5.371651000	-2.617878000	-3.318413000	Au	-3.881151000	1.826097000	0.853692000
H	-5.180316000	-2.996700000	-3.267331000	N	-3.457429000	-2.924565000	-3.377785000
H	-4.358857000	-3.311141000	-1.711741000	N	-1.571707000	-3.953661000	-3.805405000
H	-4.171269000	-1.559751000	6.054373000	N	0.931241000	-4.103464000	-3.821881000

N	2.937262000	-3.320279000	-3.417648000	C	0.849186000	-4.049437000	2.328422000
N	-4.205052000	-0.429142000	-1.037050000	C	-0.283873000	-4.199867000	3.161501000
N	4.071717000	-0.966994000	-1.077057000	C	-1.402850000	-3.911388000	2.346236000
N	4.219910000	-1.527941000	3.839274000	C	-2.878944000	-4.024060000	2.637835000
N	3.016335000	-3.294711000	3.362630000	C	-3.978127000	-1.754022000	2.814090000
N	0.433225000	-3.674906000	1.072994000	C	-4.049673000	-1.561880000	5.110055000
N	-0.965286000	-3.589937000	1.083367000	C	-3.463654000	-2.771601000	4.809396000
N	-3.429744000	-2.868640000	3.406278000	C	-1.790499000	3.682465000	-2.775484000
N	-4.357792000	-0.942670000	3.880519000	C	-2.879171000	3.471313000	-4.788637000
N	-2.961605000	3.310673000	-3.393178000	C	-1.623622000	3.969515000	-5.057272000
N	-0.961840000	4.098092000	-3.817369000	C	0.332678000	4.795589000	-3.640101000
N	1.541378000	3.961309000	-3.824962000	C	2.321937000	3.453111000	-2.787926000
N	3.428617000	2.928565000	-3.412787000	C	3.353769000	3.089337000	-4.808379000
N	-4.087964000	0.964135000	-1.042991000	C	2.169280000	3.742444000	-5.069648000
N	4.179842000	0.427681000	-1.073312000	C	-4.177819000	2.869072000	-2.648477000
N	4.401007000	0.947205000	3.845765000	C	-4.189964000	1.395687000	-2.341109000
N	3.468415000	2.872765000	3.377127000	C	4.566175000	2.303914000	-2.674652000
N	0.987130000	3.608645000	1.070420000	C	4.342821000	0.845895000	-2.370455000
N	-0.411435000	3.687574000	1.072758000	C	4.013565000	1.758038000	2.781618000
N	-2.974384000	3.297961000	3.385991000	C	4.100571000	1.566695000	5.077166000
N	-4.174632000	1.531721000	3.871590000	C	3.511898000	2.775991000	4.780123000
C	-2.345068000	-3.448126000	-2.761634000	C	2.914304000	4.029380000	2.612328000
C	-3.392005000	-3.082128000	-4.774458000	C	1.435682000	3.920695000	2.331406000
C	-2.208706000	-3.733032000	-5.045314000	C	0.323144000	4.202010000	3.158228000
C	-0.365334000	-4.793587000	-3.630874000	C	-0.816683000	4.054253000	2.334031000
C	1.771521000	-3.689893000	-2.788784000	C	-2.267844000	4.360084000	2.611748000
C	2.840760000	-3.481794000	-4.812049000	C	-3.681606000	2.273086000	2.800245000
C	1.581395000	-3.977380000	-5.068133000	C	-3.777700000	2.106108000	5.097400000
C	-4.594190000	-2.308245000	-2.631756000	C	-3.020639000	3.214742000	4.789570000
C	-4.378601000	-0.848623000	-2.332013000	C	-4.374126000	0.277488000	-3.186261000
C	4.159166000	-2.873079000	-2.684354000	C	4.337038000	-0.281198000	-3.223754000
C	4.165584000	-1.399353000	-2.376096000	C	5.106344000	-0.348325000	3.715465000
C	3.728274000	-2.275751000	2.771859000	C	-5.062873000	0.352969000	3.754374000
C	3.818900000	-2.093385000	5.068038000	H	-4.185482000	-2.761497000	-5.438170000
C	3.059666000	-3.202058000	4.765813000	H	-1.800692000	-4.079608000	-5.986835000
C	2.302775000	-4.356664000	2.594105000	H	-0.418420000	-5.609702000	-4.364282000

H	-0.383374000	-5.209164000	-2.617736000	H	5.592327000	-0.381647000	2.734303000
H	3.663374000	-3.272552000	-5.484680000	H	5.862997000	-0.405230000	4.509537000
H	1.124984000	-4.277250000	-6.003435000	H	-5.555939000	0.386159000	2.776838000
H	-4.707927000	-2.860815000	-1.688012000	H	-5.813959000	0.411317000	4.553552000
H	-5.500097000	-2.454125000	-3.237696000	H	2.593067000	-3.931544000	5.415915000
H	5.026522000	-3.146035000	-3.302655000	C	-0.691758000	-0.138362000	-1.402921000
H	4.204470000	-3.441524000	-1.744142000	C	-0.690142000	-0.004826000	0.139101000
H	4.128612000	-1.697893000	6.027554000	H	-1.714243000	-0.236795000	-1.797154000
H	2.392929000	-5.291417000	3.166194000	H	-0.217404000	0.751493000	-1.857634000
H	2.831754000	-4.477820000	1.638069000	H	-0.118379000	-1.035979000	-1.704194000
H	-0.295888000	-4.519619000	4.198461000	C	0.753463000	-0.009143000	0.694422000
H	-3.434979000	-4.080633000	1.691250000	H	-1.199631000	0.930703000	0.426093000
H	-3.082924000	-4.933456000	3.221036000	H	-1.259445000	-0.838999000	0.585484000
H	-4.300336000	-1.124925000	6.068808000	H	0.782318000	0.194648000	1.779522000
H	-3.113189000	-3.562843000	5.460331000	H	1.219574000	-0.990468000	0.511826000
H	-3.707985000	3.260025000	-5.452964000	H	1.363280000	0.755532000	0.185660000
H	-1.176733000	4.269552000	-5.997131000	<u>I,2-butadiene@PPX</u>			
H	0.374452000	5.610552000	-4.375491000	Au	-0.663999000	3.799426000	0.839630000
H	0.358324000	5.213484000	-2.628094000	Au	2.405277000	3.125964000	0.859443000
H	4.141667000	2.768302000	-5.478507000	Au	4.273668000	0.641087000	-0.795981000
H	1.754811000	4.090865000	-6.007702000	Au	-3.455705000	2.380623000	-0.837715000
H	-4.210738000	3.436566000	-1.707227000	Au	-2.462383000	-3.171210000	0.817506000
H	-5.050234000	3.147350000	-3.257301000	Au	0.622211000	-3.766090000	0.846064000
H	5.468113000	2.441218000	-3.288460000	Au	3.441895000	-2.361858000	-0.801297000
H	4.692936000	2.857366000	-1.733033000	Au	-4.258512000	-0.642967000	-0.855949000
H	4.358127000	1.130456000	6.034401000	N	-2.350015000	3.729322000	3.404179000
H	3.165572000	3.567255000	5.433232000	N	-0.257796000	4.222317000	3.828384000
H	3.125202000	4.938201000	3.194067000	N	2.191405000	3.703983000	3.843690000
H	3.463793000	4.084320000	1.661804000	N	3.878500000	2.366706000	3.443941000
H	0.343243000	4.515487000	4.196975000	N	-3.803200000	1.565228000	1.059716000
H	-2.804614000	4.480622000	1.659961000	N	4.137156000	-0.217106000	1.110697000
H	-2.354523000	5.294869000	3.184290000	N	4.511022000	0.237189000	-3.804780000
H	-4.088415000	1.715797000	6.058723000	N	3.927235000	2.296374000	-3.347637000
H	-2.557095000	3.949630000	5.435790000	N	1.586363000	3.409144000	-1.052862000
H	-4.520279000	0.285428000	-4.261190000	N	0.218616000	3.705553000	-1.061082000
H	4.473219000	-0.289383000	-4.300004000	N	-2.372797000	3.712692000	-3.377524000

N	-3.853683000	2.170920000	-3.850573000	C	-3.898960000	-2.537706000	4.781226000
N	-3.943271000	-2.375537000	3.384410000	C	-2.845230000	-3.383721000	5.049052000
N	-2.263221000	-3.715190000	3.806891000	C	-1.198255000	-4.726994000	3.629314000
N	0.185465000	-4.235390000	3.826354000	C	1.073625000	-3.924821000	2.796720000
N	2.282114000	-3.739244000	3.427065000	C	2.167469000	-3.915674000	4.818319000
N	-4.166110000	0.215049000	1.053167000	C	0.850697000	-4.230763000	5.071417000
N	3.771178000	-1.566458000	1.107319000	C	-4.939905000	-1.550493000	2.640708000
N	3.898017000	-2.165094000	-3.806022000	C	-4.444841000	-0.158766000	2.343970000
N	2.400525000	-3.696895000	-3.351615000	C	3.555813000	-3.478457000	2.692638000
N	-0.231766000	-3.686067000	-1.069814000	C	3.804723000	-2.022311000	2.401047000
N	-1.603536000	-3.403464000	-1.084487000	C	3.250435000	-2.797963000	-2.748548000
N	-3.904474000	-2.295205000	-3.412720000	C	3.448481000	-2.676840000	-5.041554000
N	-4.475696000	-0.231255000	-3.866234000	C	2.505083000	-3.638538000	-4.753792000
C	-1.137843000	3.933160000	2.786563000	C	1.520670000	-4.631783000	-2.589934000
C	-2.244930000	3.874685000	4.799805000	C	0.131769000	-4.104792000	-2.327512000
C	-0.930700000	4.187848000	5.068389000	C	-1.006442000	-4.080856000	-3.166791000
C	1.128381000	4.714279000	3.650297000	C	-2.075792000	-3.643622000	-2.352437000
C	2.870913000	3.057390000	2.812334000	C	-3.548770000	-3.531314000	-2.654967000
C	3.840369000	2.561091000	4.836655000	C	-4.232801000	-1.103969000	-2.808957000
C	2.782038000	3.405424000	5.090321000	C	-4.301955000	-0.887912000	-5.102368000
C	-3.616904000	3.472966000	2.656604000	C	-3.939341000	-2.185331000	-4.814603000
C	-3.861861000	2.017802000	2.354374000	C	-4.261429000	0.954545000	3.196187000
C	4.885868000	1.542565000	2.713462000	C	4.191293000	-0.962085000	3.253803000
C	4.393530000	0.152566000	2.407956000	C	4.975607000	-1.159389000	-3.664017000
C	4.279283000	1.110631000	-2.746140000	C	-4.934913000	1.167902000	-3.723458000
C	4.305451000	0.886884000	-5.040177000	H	-3.095022000	3.783031000	5.464494000
C	3.935130000	2.181331000	-4.750321000	H	-0.445622000	4.419313000	6.008700000
C	3.561423000	3.526976000	-2.588409000	H	1.293107000	5.517832000	4.380847000
C	2.082966000	3.644306000	-2.311280000	H	1.219718000	5.115449000	2.635305000
C	1.030377000	4.089415000	-3.145216000	H	4.568390000	2.125186000	5.509606000
C	-0.121295000	4.124169000	-2.325427000	H	2.437163000	3.834011000	6.023325000
C	-1.504739000	4.652866000	-2.609160000	H	-3.556754000	4.034401000	1.713150000
C	-3.221826000	2.806892000	-2.784654000	H	-4.438543000	3.885700000	3.259747000
C	-3.393318000	2.686529000	-5.080177000	H	5.793662000	1.509473000	3.332652000
C	-2.460167000	3.654257000	-4.780338000	H	5.118303000	2.060835000	1.771936000
C	-2.944804000	-3.089572000	2.764902000	H	4.476180000	0.404906000	-5.994848000

H	3.908089000	4.390772000	-3.173612000	C	1.076229000	0.027219000	-2.264508000
H	4.111823000	3.501445000	-1.637148000	H	-0.670063000	-0.947777000	1.736455000
H	1.103365000	4.392490000	-4.184659000	H	-1.462122000	-0.273563000	0.282147000
H	-2.016633000	4.864450000	-1.659517000	H	-0.917030000	0.823208000	1.583161000
H	-1.441584000	5.585339000	-3.188433000	H	1.266049000	-0.900611000	-2.813049000
H	-3.783116000	2.363179000	-6.037534000	H	1.572781000	0.144937000	1.014832000
H	-1.896950000	4.311846000	-5.430695000	H	1.057220000	0.960167000	-2.838304000
H	-4.620862000	-2.082033000	5.447647000	<u>1,3-butadiene@PPX</u>			
H	-2.498891000	-3.793092000	5.990058000	Au	-3.970811000	1.170864000	-0.838879000
H	-1.372796000	-5.530013000	4.358199000	Au	-3.657308000	-1.940188000	-0.832889000
H	-1.276026000	-5.128208000	2.613158000	Au	-1.181839000	-3.833888000	0.853889000
H	3.013398000	-3.841138000	5.490433000	Au	-1.940173000	3.550128000	0.845218000
H	0.358974000	-4.482370000	6.003104000	Au	3.607152000	1.921282000	-0.821711000
H	-5.158985000	-2.068643000	1.696041000	Au	3.947245000	-1.182645000	-0.815111000
H	-5.856710000	-1.517892000	3.246659000	Au	1.936867000	-3.559856000	0.857086000
H	4.371525000	-3.895789000	3.300679000	Au	1.174604000	3.882154000	0.846802000
H	3.504841000	-4.032933000	1.744517000	N	-3.494913000	2.788764000	-3.394455000
H	3.853768000	-2.357400000	-5.993803000	N	-4.309599000	0.807193000	-3.845927000
H	1.946341000	-4.292721000	-5.411370000	N	-4.059335000	-1.670502000	-3.840232000
H	1.464870000	-5.567368000	-3.165000000	N	-2.858421000	-3.443010000	-3.380507000
H	2.019798000	-4.837813000	-1.632381000	N	-1.085886000	3.726359000	-1.060720000
H	-1.058566000	-4.383872000	-4.207485000	N	-0.308355000	-3.858317000	-1.050682000
H	-4.116458000	-3.514174000	-1.713593000	N	-0.833597000	-4.249272000	3.852508000
H	-3.883739000	-4.390939000	-3.252738000	N	-2.830913000	-3.465799000	3.412088000
H	-4.482258000	-0.406555000	-6.055631000	N	-3.842163000	-1.084749000	1.073592000
H	-3.744984000	-3.022701000	-5.473135000	N	-3.983497000	0.307857000	1.071570000
H	-4.433111000	0.995144000	4.266640000	N	-3.478732000	2.850056000	3.403817000
H	4.342172000	-1.005773000	4.327245000	N	-1.676778000	4.014994000	3.844607000
H	5.429317000	-1.275555000	-2.673615000	N	2.854929000	3.434851000	-3.379924000
H	5.724388000	-1.352620000	-4.444055000	N	4.044718000	1.650684000	-3.822153000
H	-5.398999000	1.281900000	-2.737839000	N	4.298860000	-0.824920000	-3.818198000
H	-5.676184000	1.365800000	-4.509364000	N	3.497264000	-2.812460000	-3.369861000
H	3.724069000	3.015411000	-5.407868000	N	0.306513000	3.874718000	-1.058452000
C	0.890735000	0.022197000	-0.949046000	N	1.085753000	-3.732269000	-1.047841000
C	0.698114000	0.029151000	0.364295000	N	1.651757000	-4.009012000	3.856354000
C	-0.670320000	-0.099826000	1.026309000	N	3.458098000	-2.849110000	3.422391000

N	3.959690000	-0.311582000	1.089082000	C	1.540345000	-3.977905000	-2.319398000
N	3.813973000	1.078307000	1.085518000	C	2.401095000	-3.478535000	2.808063000
N	2.804191000	3.474894000	3.409936000	C	2.250664000	-3.704378000	5.097267000
N	0.807565000	4.261822000	3.847943000	C	3.384154000	-2.971491000	4.821798000
C	-3.937826000	1.635750000	-2.790470000	C	4.546131000	-2.153681000	2.672217000
C	-3.578067000	2.697020000	-4.795534000	C	4.237842000	-0.709402000	2.373433000
C	-4.093249000	1.451891000	-5.081854000	C	4.267969000	0.429175000	3.211582000
C	-4.967178000	-0.510402000	-3.697880000	C	4.003200000	1.532435000	2.367553000
C	-3.530489000	-2.403962000	-2.781156000	C	4.007975000	3.011248000	2.657261000
C	-2.954927000	-3.373833000	-4.781991000	C	1.644343000	3.888834000	2.797990000
C	-3.713173000	-2.261346000	-5.073591000	C	1.454912000	4.074774000	5.087762000
C	-3.015355000	3.980448000	-2.633776000	C	2.708975000	3.576863000	4.809818000
C	-1.537441000	3.955779000	-2.338141000	C	-0.433083000	4.247228000	-3.170469000
C	-2.147172000	-4.509683000	-2.616437000	C	0.436835000	-4.265508000	-3.154838000
C	-0.704195000	-4.187044000	-2.324629000	C	0.485082000	-4.904256000	3.692154000
C	-1.661460000	-3.857054000	2.802633000	C	-0.510649000	4.914460000	3.685984000
C	-1.494113000	-4.092704000	5.089418000	H	-3.306156000	3.512750000	-5.453758000
C	-2.748919000	-3.597284000	4.810507000	H	-4.350794000	1.003197000	-6.033340000
C	-4.034928000	-3.009014000	2.656234000	H	-5.742278000	-0.590351000	-4.471930000
C	-4.033878000	-1.531890000	2.358128000	H	-5.429085000	-0.554684000	-2.705667000
C	-4.298641000	-0.424622000	3.196672000	H	-2.520302000	-4.118683000	-5.436881000
C	-4.262877000	0.710711000	2.354527000	H	-4.054178000	-1.877168000	-6.027080000
C	-4.564690000	2.157498000	2.648739000	H	-3.577475000	4.011832000	-1.689258000
C	-2.414874000	3.473645000	2.794185000	H	-3.272154000	4.870823000	-3.225451000
C	-2.288353000	3.722218000	5.082066000	H	-2.220382000	-5.436227000	-3.203866000
C	-3.419222000	2.986644000	4.802769000	H	-2.689736000	-4.649662000	-1.670428000
C	3.515057000	2.394827000	-2.769413000	H	-1.047821000	-4.374614000	6.035159000
C	2.955670000	3.355331000	-4.781048000	H	-4.917620000	-3.281907000	3.252203000
C	3.707224000	2.235954000	-5.062250000	H	-4.059935000	-3.571435000	1.711725000
C	4.955221000	0.493395000	-3.668616000	H	-4.525438000	-0.446235000	4.257511000
C	3.943671000	-1.662637000	-2.762568000	H	-4.703383000	2.700849000	1.703087000
C	3.561802000	-2.711139000	-4.771831000	H	-5.484703000	2.246283000	3.244231000
C	4.069748000	-1.462939000	-5.056799000	H	-1.903672000	4.081638000	6.028656000
C	2.148023000	4.510195000	-2.625276000	H	-4.181942000	2.593374000	5.463413000
C	0.704487000	4.190879000	-2.333245000	H	2.531138000	4.100186000	-5.442533000
C	3.019020000	-4.005338000	-2.611076000	H	4.055614000	1.846995000	-6.011218000

H	5.735570000	0.572666000	-4.437470000	Au	1.565076000	-3.437811000	-0.831205000
H	5.407948000	0.541067000	-2.672361000	Au	3.999014000	-1.530662000	0.848175000
H	3.287143000	-3.524620000	-5.431733000	Au	-4.058649000	-1.576106000	0.824293000
H	4.320863000	-1.010027000	-6.008057000	Au	-1.602201000	3.481346000	-0.839999000
H	2.690226000	4.654021000	-1.679781000	Au	1.537649000	3.447030000	-0.832994000
H	2.224547000	5.432071000	-3.219649000	Au	3.987164000	1.557724000	0.845964000
H	3.277505000	-4.895559000	-3.202317000	Au	-4.071881000	1.549387000	0.824379000
H	3.579243000	-4.034077000	-1.665514000	N	-3.195501000	-3.140580000	-3.419454000
H	1.856792000	-4.054692000	6.043456000	N	-1.234887000	-4.033037000	-3.816578000
H	4.140376000	-2.571522000	5.485782000	N	1.273356000	-4.019017000	-3.808127000
H	5.462459000	-2.236913000	3.274177000	N	3.224409000	-3.113551000	-3.394927000
H	4.693228000	-2.698133000	1.728408000	N	-4.156604000	-0.712917000	-1.081964000
H	4.496501000	0.455696000	4.272002000	N	4.149538000	-0.685120000	-1.061133000
H	4.035698000	3.568320000	1.709728000	N	4.306458000	-1.220829000	3.864691000
H	4.890482000	3.284854000	3.253262000	N	3.221178000	-3.059987000	3.382687000
H	1.001651000	4.339631000	6.035125000	N	0.684470000	-3.549571000	1.078461000
H	3.529024000	3.329888000	5.472538000	N	-0.716261000	-3.559755000	1.074883000
H	-0.458095000	4.502954000	-4.224617000	N	-3.268324000	-3.088188000	3.365771000
H	0.463758000	-4.533768000	-4.205862000	N	-4.367041000	-1.254165000	3.839787000
H	0.529343000	-5.344419000	2.690144000	N	-3.222989000	3.120686000	-3.419677000
H	0.559470000	-5.697414000	4.448317000	N	-1.267797000	4.024427000	-3.817738000
H	-0.552955000	5.357015000	2.684908000	N	1.240438000	4.022602000	-3.810270000
H	-0.591401000	5.705068000	4.444192000	N	3.196946000	3.128491000	-3.397728000
H	-3.576857000	-3.370079000	5.470631000	N	-4.163103000	0.685904000	-1.081985000
C	0.377376000	0.000506000	-1.322988000	N	4.143147000	0.709711000	-1.062137000
C	-0.413833000	-0.023228000	-0.076778000	N	4.298193000	1.254831000	3.863064000
C	0.485200000	0.072032000	1.190839000	N	3.199358000	3.085287000	3.378766000
C	1.059632000	0.026726000	-2.348172000	N	0.656683000	3.554545000	1.076356000
H	-0.147835000	0.068147000	2.094835000	N	-0.744083000	3.555436000	1.073785000
H	1.080585000	0.997451000	1.170336000	N	-3.290813000	3.065810000	3.366082000
H	1.182235000	-0.779382000	1.231942000	N	-4.375967000	1.223636000	3.839949000
H	1.649185000	0.052462000	-3.239655000	C	-2.048209000	-3.559722000	-2.787886000
H	-1.005370000	-0.955281000	-0.038835000	C	-3.113767000	-3.330257000	-4.811156000
H	-1.130330000	0.817789000	-0.085935000	C	-1.882613000	-3.894903000	-5.062815000
<u>2-butyne@PPX</u>				C	0.023039000	-4.786948000	-3.614022000
Au	-1.573560000	-3.490526000	-0.839113000	C	2.069541000	-3.527993000	-2.773296000

C	3.162563000	-3.320316000	-4.785359000	C	-3.924768000	1.997458000	2.773894000
C	1.937594000	-3.893038000	-5.047207000	C	-4.026866000	1.820488000	5.069682000
C	-4.383715000	-2.611408000	-2.685984000	C	-3.341791000	2.977229000	4.769108000
C	-4.285117000	-1.140420000	-2.379932000	C	-4.375056000	-0.014522000	-3.230070000
C	4.407971000	-2.585215000	-2.652768000	C	4.409035000	0.012072000	-3.204041000
C	4.309759000	-1.114007000	-2.354077000	C	5.104437000	0.019614000	3.741558000
C	3.857853000	-1.991442000	2.795044000	C	-5.171799000	-0.018105000	3.712041000
C	3.951565000	-1.819424000	5.092059000	H	-3.926746000	-3.089049000	-5.484860000
C	3.266735000	-2.974863000	4.786209000	H	-1.445596000	-4.233181000	-5.994323000
C	2.575445000	-4.158188000	2.605881000	H	0.030300000	-5.620910000	-4.328985000
C	1.110391000	-3.930790000	2.328213000	H	0.022136000	-5.180657000	-2.592090000
C	-0.018149000	-4.176544000	3.144966000	H	3.984465000	-3.084844000	-5.450204000
C	-1.145450000	-3.944211000	2.323996000	H	1.515234000	-4.245284000	-5.980331000
C	-2.610035000	-4.184180000	2.595207000	H	-4.465460000	-3.174328000	-1.744952000
C	-3.909395000	-2.024131000	2.773652000	H	-5.268793000	-2.824234000	-3.302699000
C	-4.014761000	-1.849256000	5.069469000	H	5.297733000	-2.804297000	-3.260299000
C	-3.321144000	-3.000863000	4.768794000	H	4.477659000	-3.143224000	-1.707777000
C	-2.078071000	3.546870000	-2.788563000	H	4.242269000	-1.411186000	6.052218000
C	-3.142848000	3.310333000	-4.811448000	H	2.710968000	-5.088062000	3.176623000
C	-1.915116000	3.882122000	-5.063722000	H	3.118929000	-4.246069000	1.654385000
C	-0.013534000	4.784680000	-3.616246000	H	-0.017851000	-4.524045000	4.173143000
C	2.040512000	3.537602000	-2.775497000	H	-3.148915000	-4.280011000	1.641950000
C	3.132513000	3.332945000	-4.788412000	H	-2.741161000	-5.113224000	3.168415000
C	1.904117000	3.898384000	-5.049866000	H	-4.310842000	-1.440571000	6.027800000
C	-4.406907000	2.582245000	-2.685994000	H	-2.906761000	-3.760727000	5.419558000
C	-4.295661000	1.112144000	-2.379856000	H	-3.954602000	3.063949000	-5.484759000
C	4.385156000	2.609992000	-2.655999000	H	-1.480323000	4.222524000	-5.995501000
C	4.299411000	1.138373000	-2.355598000	H	-0.010644000	5.618016000	-4.331974000
C	3.843927000	2.020787000	2.792381000	H	-0.015907000	5.179305000	-2.594666000
C	3.938501000	1.852073000	5.089680000	H	3.954986000	3.101050000	-5.453805000
C	3.245137000	3.002005000	4.782381000	H	1.478756000	4.246679000	-5.983108000
C	2.544961000	4.177580000	2.600998000	H	-4.493144000	3.144544000	-1.744988000
C	1.081159000	3.939488000	2.325445000	H	-5.293752000	2.787574000	-3.302697000
C	-0.048348000	4.178291000	3.142951000	H	5.272627000	2.835631000	-3.264494000
C	-1.174759000	3.937624000	2.323080000	H	4.451180000	3.169625000	-1.711702000
C	-2.640834000	4.166975000	2.595656000	H	4.231733000	1.446895000	6.050365000

H	2.828048000	3.764053000	5.428834000	N	1.926404000	3.901811000	3.861010000
H	2.674590000	5.109349000	3.170046000	N	3.633802000	2.601352000	3.424585000
H	3.086834000	4.267755000	1.648777000	N	-3.776558000	1.354304000	1.046348000
H	-0.049705000	4.526486000	4.170894000	N	3.944256000	0.014793000	1.103870000
H	-3.181053000	4.259488000	1.642842000	N	4.347846000	0.505898000	-3.802070000
H	-2.778120000	5.094698000	3.169527000	N	3.690805000	2.548149000	-3.363398000
H	-4.319426000	1.409291000	6.028020000	N	1.361007000	3.716109000	-1.048817000
H	-2.932569000	3.739768000	5.420016000	N	-0.017926000	3.957335000	-1.058156000
H	-4.514162000	-0.015124000	-4.306012000	N	-2.574007000	3.648880000	-3.400899000
H	4.570211000	0.012040000	-4.276893000	N	-3.872010000	1.945830000	-3.857246000
H	5.596867000	0.020714000	2.762941000	N	-3.706171000	-2.592277000	3.375906000
H	5.857734000	0.022621000	4.540610000	N	-1.992401000	-3.877940000	3.831024000
H	-5.656957000	-0.019813000	2.729954000	N	0.468544000	-4.299469000	3.856088000
H	-5.931380000	-0.020946000	4.505219000	N	2.522596000	-3.663396000	3.437160000
H	2.855723000	-3.739356000	5.433672000	N	-4.042595000	-0.018687000	1.042712000
C	0.868314000	0.005318000	0.688150000	N	3.709351000	-1.364552000	1.109317000
C	0.821911000	0.003794000	-0.541203000	N	3.925639000	-1.950479000	-3.797298000
C	0.717533000	-0.000302000	-2.010110000	N	2.619366000	-3.651853000	-3.356312000
C	0.909937000	0.006398000	2.160219000	N	0.026422000	-3.944646000	-1.051940000
H	1.715311000	-0.030642000	-2.477752000	N	-1.352301000	-3.702462000	-1.065428000
H	0.199913000	0.911072000	-2.361108000	N	-3.644109000	-2.553058000	-3.412788000
H	0.407859000	0.902810000	2.564324000	N	-4.292496000	-0.510672000	-3.862703000
H	1.953435000	0.008891000	2.515788000	C	-1.388011000	4.010305000	2.789548000
H	0.151791000	-0.886599000	-2.351248000	C	-2.475442000	3.731442000	4.794204000
H	0.412813000	-0.892212000	2.565409000	C	-1.194338000	4.147951000	5.082051000
<u>C₄H₈@PPX</u>				C	0.827680000	4.880525000	3.701366000
Au	-0.910124000	4.006082000	0.840404000	C	2.633618000	3.318826000	2.811293000
Au	2.190978000	3.459859000	0.859105000	C	3.566009000	2.721601000	4.824626000
Au	3.990556000	0.887736000	-0.803143000	C	2.494957000	3.542352000	5.101559000
Au	-3.468710000	2.193199000	-0.849200000	C	-3.803398000	3.285018000	2.633662000
Au	-2.219152000	-3.444964000	0.827089000	C	-3.911828000	1.811512000	2.334498000
Au	0.890078000	-3.967934000	0.857522000	C	4.662742000	1.821890000	2.674697000
Au	3.504511000	-2.218718000	-0.794337000	C	4.249879000	0.401245000	2.386123000
Au	-4.053512000	-0.906961000	-0.855252000	C	4.036718000	1.365920000	-2.751389000
N	-2.572518000	3.656745000	3.392607000	C	4.190065000	1.160461000	-5.042329000
N	-0.533263000	4.314677000	3.846998000	C	3.773610000	2.443453000	-4.764535000

C	3.309520000	3.780037000	-2.613158000	H	0.953555000	5.657141000	4.467821000
C	1.832605000	3.880151000	-2.327730000	H	0.908471000	5.327682000	2.704848000
C	0.754524000	4.227075000	-3.174958000	H	4.285490000	2.258137000	5.488170000
C	-0.387787000	4.271660000	-2.342710000	H	2.128390000	3.918433000	6.048817000
C	-1.806755000	4.680134000	-2.643725000	H	-3.789157000	3.848448000	1.689699000
C	-3.298348000	2.646686000	-2.798101000	H	-4.665645000	3.619962000	3.228321000
C	-3.498667000	2.518218000	-5.091506000	H	5.585545000	1.839906000	3.272305000
C	-2.679444000	3.586766000	-4.802275000	H	4.847226000	2.347417000	1.726844000
C	-2.696231000	-3.305347000	2.772840000	H	4.420654000	0.690131000	-5.990225000
C	-3.647198000	-2.704959000	4.777180000	H	3.644218000	4.642430000	-3.207561000
C	-2.572457000	-3.516415000	5.065616000	H	3.864218000	3.770206000	-1.664012000
C	-0.892606000	-4.858081000	3.685688000	H	0.802013000	4.454046000	-4.234887000
C	1.341311000	-3.990962000	2.814083000	H	-2.342104000	4.861837000	-1.700757000
C	2.406456000	-3.756194000	4.836087000	H	-1.823302000	5.603630000	-3.240282000
C	1.116321000	-4.159483000	5.101695000	H	-3.865908000	2.155930000	-6.043829000
C	-4.738713000	-1.825157000	2.618937000	H	-2.208560000	4.308519000	-5.458029000
C	-4.332054000	-0.403390000	2.327659000	H	-4.375283000	-2.244082000	5.433062000
C	3.766231000	-3.292343000	2.697839000	H	-2.210215000	-3.885314000	6.017291000
C	3.866219000	-1.819638000	2.395567000	H	-1.033329000	-5.636985000	4.447273000
C	3.362567000	-2.668480000	-2.744963000	H	-0.958730000	-5.301973000	2.686622000
C	3.529848000	-2.494777000	-5.037424000	H	3.236013000	-3.569847000	5.506806000
C	2.705305000	-3.562077000	-4.758040000	H	0.635732000	-4.388937000	6.044753000
C	1.841380000	-4.680761000	-2.606363000	H	-4.913967000	-2.356120000	1.672259000
C	0.416884000	-4.272059000	-2.327770000	H	-5.664046000	-1.849639000	3.212457000
C	-0.713449000	-4.239612000	-3.176302000	H	4.619221000	-3.620393000	3.309034000
C	-1.803883000	-3.883672000	-2.349085000	H	3.769479000	-3.859107000	1.755747000
C	-3.275753000	-3.787269000	-2.658535000	H	3.888326000	-2.118102000	-5.987445000
C	-4.009840000	-1.374176000	-2.806657000	H	2.220680000	-4.267714000	-5.421251000
C	-4.098605000	-1.160030000	-5.099841000	H	1.866374000	-5.606827000	-3.198640000
C	-3.687527000	-2.443272000	-4.814632000	H	2.363713000	-4.856702000	-1.655190000
C	-4.258561000	0.727353000	3.173769000	H	-0.745911000	-4.482136000	-4.233391000
C	4.204070000	-0.731019000	3.232144000	H	-3.847644000	-3.781127000	-1.719576000
C	4.908964000	-0.854538000	-3.645022000	H	-3.599394000	-4.647963000	-3.261397000
C	-4.856955000	0.849795000	-3.717479000	H	-4.299469000	-0.685394000	-6.052352000
H	-3.311079000	3.525377000	5.451455000	H	-3.466204000	-3.272803000	-5.474605000
H	-0.728480000	4.369506000	6.034315000	H	-4.470682000	0.764700000	4.237219000

H	4.426890000	-0.765367000	4.293481000	N	-4.095314000	-0.740940000	-1.100672000
H	5.353904000	-0.929929000	-2.647047000	N	-3.123042000	-3.164148000	-3.431206000
H	5.685806000	-0.989303000	-4.409861000	N	-1.161711000	-4.056821000	-3.819240000
H	-5.320287000	0.927123000	-2.728086000	N	3.255742000	-3.053774000	3.406878000
H	-5.621061000	0.983099000	-4.495216000	N	4.305734000	-1.192926000	3.885494000
H	3.575031000	3.276346000	-5.427514000	N	4.273614000	1.287226000	3.887569000
H	-0.807226000	0.320185000	2.100353000	N	3.173793000	3.119979000	3.412510000
C	-0.595792000	-0.294085000	1.208163000	N	0.746967000	-3.563634000	1.090912000
C	0.407238000	0.413261000	0.260441000	N	0.646845000	3.561500000	1.100408000
C	0.632538000	-0.393151000	-1.005384000	N	1.231679000	4.078063000	-3.783236000
C	0.821065000	0.130787000	-2.241034000	N	3.187284000	3.183346000	-3.370040000
H	-0.193054000	-1.269913000	1.536851000	N	4.089065000	0.753404000	-1.038295000
H	-1.546341000	-0.480998000	0.686161000	N	4.108756000	-0.644204000	-1.037690000
H	1.375443000	0.544970000	0.780971000	N	3.279146000	-3.096198000	-3.373352000
H	0.043962000	1.419465000	-0.000494000	N	1.344849000	-4.031432000	-3.795714000
H	0.649529000	-1.481000000	-0.873774000	C	-3.865946000	-2.061025000	2.754469000
H	0.800817000	1.211564000	-2.408211000	C	-3.292150000	-3.047586000	4.748257000
H	1.005290000	-0.509765000	-3.108552000	C	-3.993444000	-1.900816000	5.049604000
<u>(E)-C₄H₈@PPX</u>				C	-5.152521000	-0.071471000	3.691113000
Au	-3.987552000	-1.596166000	0.806647000	C	-3.923510000	1.957796000	2.763354000
Au	-4.036218000	1.503118000	0.812577000	C	-3.369945000	2.947026000	4.761595000
Au	-1.592465000	3.434581000	-0.835396000	C	-4.039874000	1.780303000	5.057766000
Au	-1.491220000	-3.459412000	-0.848211000	C	-2.557518000	-4.214525000	2.573238000
Au	3.981398000	-1.499284000	0.869930000	C	-1.091843000	-3.967728000	2.316341000
Au	3.953742000	1.602094000	0.871820000	C	-2.668141000	4.143059000	2.591220000
Au	1.526181000	3.501292000	-0.807863000	C	-1.198213000	3.928731000	2.329212000
Au	1.626313000	-3.478630000	-0.814875000	C	-2.072341000	3.536208000	-2.782425000
N	-3.226941000	-3.126332000	3.345267000	C	-1.928402000	3.938170000	-5.048794000
N	-4.337327000	-1.300029000	3.820343000	C	-3.147425000	3.345035000	-4.805650000
N	-4.371238000	1.178117000	3.825758000	C	-4.393158000	2.554006000	-2.693386000
N	-3.310879000	3.035894000	3.358934000	C	-4.259994000	1.084801000	-2.393844000
N	-0.652521000	-3.571644000	1.075239000	C	-4.330224000	-0.041181000	-3.245992000
N	-0.753356000	3.540830000	1.087426000	C	-4.225916000	-1.167714000	-2.398353000
N	-1.275354000	4.053413000	-3.802788000	C	-4.314884000	-2.639112000	-2.702545000
N	-3.216397000	3.115571000	-3.419211000	C	-1.968573000	-3.559436000	-2.796593000
N	-4.116488000	0.657293000	-1.098164000	C	-1.818913000	-3.953770000	-5.064161000

C	-3.050800000	-3.389234000	-4.818233000	H	-3.202677000	4.230209000	1.634590000
C	3.854551000	-1.964406000	2.817820000	H	-1.503085000	4.309676000	-5.973050000
C	3.325437000	-2.979583000	4.809814000	H	-5.281319000	2.747357000	-3.311920000
C	3.988539000	-1.810801000	5.113419000	H	-4.492395000	3.108923000	-1.749260000
C	5.087271000	0.057584000	3.758429000	H	-4.473023000	-0.041230000	-4.321371000
C	3.809349000	2.052829000	2.821503000	H	-4.396490000	-3.199842000	-1.760163000
C	3.234404000	3.038410000	4.815417000	H	-5.197526000	-2.857042000	-3.320834000
C	3.928949000	1.887435000	5.116814000	H	-1.386289000	-4.313342000	-5.989766000
C	2.627244000	-4.164459000	2.631759000	H	-3.869924000	-3.169074000	-5.491677000
C	1.162961000	-3.950935000	2.342288000	H	2.941697000	-3.757611000	5.457894000
C	2.514895000	4.213667000	2.638948000	H	4.284523000	-1.402524000	6.071957000
C	1.056468000	3.960961000	2.350474000	H	5.847892000	0.066516000	4.550484000
C	2.033591000	3.601028000	-2.748253000	H	5.571852000	0.064808000	2.776036000
C	1.890308000	3.942726000	-5.023734000	H	2.822872000	3.800460000	5.465409000
C	3.118602000	3.376503000	-4.762071000	H	4.228716000	1.481259000	6.075057000
C	4.370067000	2.655747000	-2.626870000	H	3.178241000	-4.251921000	1.684472000
C	4.277346000	1.183156000	-2.327862000	H	2.769753000	-5.088975000	3.209180000
C	4.420450000	0.058350000	-3.171828000	H	2.631431000	5.141098000	3.217591000
C	4.310247000	-1.069332000	-2.326743000	H	3.063481000	4.318110000	1.691946000
C	4.445025000	-2.538808000	-2.625737000	H	1.462004000	4.283449000	-5.958366000
C	2.136503000	-3.548963000	-2.755794000	H	3.937939000	3.137213000	-5.428654000
C	1.998610000	-3.865610000	-5.035104000	H	5.260799000	2.875502000	-3.232616000
C	3.213469000	-3.273704000	-4.767624000	H	4.437342000	3.214525000	-1.682251000
C	0.028181000	-4.204409000	3.146541000	H	4.609928000	0.060595000	-4.240018000
C	-0.081970000	4.190540000	3.156533000	H	4.524547000	-3.096154000	-1.681293000
C	-0.030968000	4.825779000	-3.589871000	H	5.343475000	-2.733216000	-3.228763000
C	0.097727000	-4.805877000	-3.610216000	H	1.577433000	-4.205096000	-5.973422000
H	-2.879588000	-3.809406000	5.397845000	H	4.026107000	-3.006703000	-5.431877000
H	-4.299612000	-1.498905000	6.007604000	H	0.019185000	-4.557461000	4.172748000
H	-5.916451000	-0.083815000	4.479994000	H	-0.096690000	4.545069000	4.182184000
H	-5.632330000	-0.075684000	2.706312000	H	-0.042203000	5.213036000	-2.565339000
H	-2.975623000	3.715395000	5.414791000	H	-0.034162000	5.663957000	-4.299909000
H	-4.332601000	1.364645000	6.014106000	H	0.092669000	-5.201482000	-2.588818000
H	-3.087377000	-4.307689000	1.614509000	H	0.111807000	-5.638200000	-4.326962000
H	-2.688937000	-5.147138000	3.140394000	H	-3.960459000	3.107741000	-5.480643000
H	-2.817660000	5.069391000	3.164091000	H	1.309669000	0.888068000	-2.349351000

C	0.813933000	-0.036863000	-2.006070000	N	-4.258499000	-0.238307000	-1.036782000
C	0.606374000	-0.006093000	-0.505488000	N	3.786720000	1.559418000	-1.068842000
C	-0.598455000	-0.077676000	0.115022000	N	3.870525000	2.219967000	3.845498000
C	-0.774223000	-0.037437000	1.619575000	N	2.365128000	3.733590000	3.355287000
H	-0.147413000	-0.146082000	-2.536857000	N	-0.232311000	3.611218000	1.070291000
H	1.474345000	-0.872901000	-2.291917000	N	-1.599309000	3.304902000	1.074921000
H	1.512716000	0.083767000	0.106569000	N	-3.945613000	2.299383000	3.389246000
H	-1.513017000	-0.176373000	-0.482356000	N	-4.515078000	0.244670000	3.885553000
H	0.204635000	0.012329000	2.126828000	C	-1.085054000	-3.856191000	-2.741387000
H	-1.311914000	-0.936338000	1.969221000	C	-2.202652000	-3.900110000	-4.750237000
H	-1.367766000	0.845665000	1.916161000	C	-0.883525000	-4.194360000	-5.014273000
<u>(Z)-C₄H₈@PPX</u>				C	1.177590000	-4.667756000	-3.583478000
Au	-0.608751000	-3.654467000	-0.800869000	C	2.944751000	-3.039392000	-2.752670000
Au	2.466799000	-3.075734000	-0.803465000	C	3.913583000	-2.548080000	-4.777262000
Au	4.324557000	-0.609267000	0.863197000	C	2.842498000	-3.376737000	-5.030194000
Au	-3.462039000	-2.347574000	0.874078000	C	-3.576922000	-3.480537000	-2.613513000
Au	-2.421943000	2.989277000	-0.840571000	C	-3.866270000	-2.033024000	-2.322969000
Au	0.624529000	3.690990000	-0.842991000	C	4.967472000	-1.540998000	-2.649855000
Au	3.445383000	2.376621000	0.831518000	C	4.466538000	-0.153973000	-2.348056000
Au	-4.376964000	0.625581000	0.866072000	C	4.301728000	-1.053879000	2.818004000
N	-2.304354000	-3.705598000	-3.360021000	C	4.332204000	-0.825291000	5.110450000
N	-0.203867000	-4.168524000	-3.776936000	C	3.978964000	-2.125725000	4.823657000
N	2.252586000	-3.672106000	-3.782438000	C	3.606839000	-3.477424000	2.661714000
N	3.959841000	-2.361301000	-3.383664000	C	2.131394000	-3.583762000	2.367606000
N	-3.862078000	-1.578788000	-1.028973000	C	1.071716000	-4.035236000	3.186624000
N	4.178443000	0.216024000	-1.058184000	C	-0.077327000	-4.040678000	2.361973000
N	4.522532000	-0.174142000	3.873600000	C	-1.460831000	-4.575280000	2.632446000
N	3.966549000	-2.243121000	3.421841000	C	-3.205863000	-2.758358000	2.820538000
N	1.642081000	-3.316634000	1.110666000	C	-3.380812000	-2.656709000	5.116981000
N	0.269563000	-3.596209000	1.108612000	C	-2.427515000	-3.602707000	4.811325000
N	-2.338185000	-3.649879000	3.408076000	C	-2.936900000	2.966730000	-2.781771000
N	-3.851851000	-2.142991000	3.890325000	C	-3.978353000	2.543599000	-4.787703000
N	-3.981093000	2.318905000	-3.398814000	C	-2.906172000	3.366190000	-5.053320000
N	-2.272230000	3.621083000	-3.817841000	C	-1.198825000	4.620233000	-3.628772000
N	0.184298000	4.127204000	-3.825141000	C	1.077355000	3.847696000	-2.791845000
N	2.289593000	3.677585000	-3.418411000	C	2.172294000	3.829717000	-4.812383000

C	0.849708000	4.116079000	-5.070033000	H	-3.778040000	-2.347826000	6.076108000
C	-4.991926000	1.513496000	-2.654261000	H	-1.850755000	-4.252224000	5.457846000
C	-4.499629000	0.127639000	-2.336723000	H	-4.736417000	2.141346000	-5.448381000
C	3.565550000	3.454968000	-2.676637000	H	-2.576774000	3.807137000	-5.986165000
C	3.839718000	2.008625000	-2.364488000	H	-1.367536000	5.431346000	-4.349990000
C	3.223263000	2.828951000	2.773220000	H	-1.276690000	5.013359000	-2.609413000
C	3.411048000	2.751237000	5.069064000	H	3.019612000	3.760697000	-5.483363000
C	2.462835000	3.700981000	4.758507000	H	0.353204000	4.342960000	-6.005523000
C	1.481866000	4.650846000	2.574370000	H	-5.216060000	2.044487000	-1.717664000
C	0.101501000	4.104261000	2.310322000	H	-5.902681000	1.478364000	-3.268885000
C	-1.052118000	4.111615000	3.126797000	H	4.375425000	3.878073000	-3.288258000
C	-2.100021000	3.614454000	2.317471000	H	3.500167000	4.022678000	-1.737337000
C	-3.577907000	3.514402000	2.603411000	H	3.811835000	2.450602000	6.029338000
C	-4.306489000	1.104719000	2.811498000	H	1.894548000	4.361636000	5.401283000
C	-4.293987000	0.913335000	5.107520000	H	1.412522000	5.593041000	3.136678000
C	-3.932404000	2.204969000	4.792685000	H	1.986450000	4.848790000	1.618030000
C	-4.261014000	-0.980654000	-3.180338000	H	-1.128737000	4.471940000	4.147637000
C	4.261778000	0.952213000	-3.202776000	H	-4.133699000	3.474340000	1.655652000
C	4.965355000	1.229904000	3.726703000	H	-3.914883000	4.391579000	3.173949000
C	-4.955199000	-1.162700000	3.769512000	H	-4.443973000	0.443387000	6.071670000
H	-3.057749000	-3.851423000	-5.413089000	H	-3.709160000	3.047911000	5.434688000
H	-0.397853000	-4.450447000	-5.947918000	H	-4.393353000	-1.025039000	-4.256137000
H	1.338885000	-5.483071000	-4.301580000	H	4.430079000	0.992582000	-4.273715000
H	1.258213000	-5.055198000	-2.562142000	H	5.430485000	1.344545000	2.741388000
H	4.645441000	-2.120157000	-5.451191000	H	5.701393000	1.441421000	4.513983000
H	2.488269000	-3.797092000	-5.963396000	H	-5.433902000	-1.297452000	2.793299000
H	-3.501366000	-4.030991000	-1.664829000	H	-5.678314000	-1.364448000	4.571127000
H	-4.385886000	-3.923366000	-3.212748000	H	3.777842000	-2.960397000	5.483563000
H	5.876651000	-1.505269000	-3.266643000	C	-0.611582000	0.007542000	0.120878000
H	5.196799000	-2.060751000	-1.708483000	C	-0.671300000	-0.139416000	-1.229105000
H	4.496047000	-0.338586000	6.063989000	H	-1.560507000	0.112883000	0.658764000
H	3.941650000	-4.339787000	3.255498000	H	-1.661348000	-0.137265000	-1.695527000
H	4.169722000	-3.458257000	1.717589000	C	0.643001000	0.061148000	0.969362000
H	1.137045000	-4.360410000	4.219945000	H	0.704759000	1.027475000	1.502814000
H	-1.966816000	-4.778586000	1.677935000	H	0.640566000	-0.746151000	1.723251000
H	-1.395380000	-5.514271000	3.200974000	H	1.555570000	-0.045792000	0.366757000

C	0.503824000	-0.309805000	-2.176602000	N	1.257735000	-3.957678000	-3.780638000
H	1.473659000	-0.307734000	-1.658022000	C	-3.932387000	-2.012530000	2.794374000
H	0.416587000	-1.270970000	-2.716749000	C	-3.233686000	-2.949287000	4.773509000
H	0.514064000	0.496606000	-2.934069000	C	-3.938573000	-1.809672000	5.091039000
<u>Isobutylene@PPX</u>				C	-5.167836000	-0.002817000	3.769507000
Au	-4.192085000	-1.581489000	0.850465000	C	-3.934999000	2.008548000	2.794442000
Au	-4.194391000	1.577317000	0.850492000	C	-3.237426000	2.946033000	4.773642000
Au	-1.574924000	3.381330000	-0.811236000	C	-3.940939000	1.805559000	5.091109000
Au	-1.570713000	-3.381184000	-0.811493000	C	-2.585237000	-4.145608000	2.592776000
Au	4.121156000	-1.572321000	0.850061000	C	-1.114756000	-3.921313000	2.335033000
Au	4.118681000	1.575495000	0.850379000	C	-2.590158000	4.143186000	2.593094000
Au	1.610863000	3.492354000	-0.796812000	C	-1.119440000	3.920299000	2.335406000
Au	1.614821000	-3.490582000	-0.797177000	C	-2.075719000	3.476111000	-2.754536000
N	-3.240020000	-3.053535000	3.370807000	C	-1.921623000	3.836886000	-5.028815000
N	-4.357562000	-1.238007000	3.871562000	C	-3.159941000	3.291348000	-4.774606000
N	-4.359207000	1.233448000	3.871589000	C	-4.440715000	2.595720000	-2.653669000
N	-3.243876000	3.050356000	3.370953000	C	-4.387569000	1.123182000	-2.344831000
N	-0.678408000	-3.528519000	1.092069000	C	-4.390008000	-0.002476000	-3.200137000
N	-0.682744000	3.528482000	1.092270000	C	-4.386429000	-1.128007000	-2.344674000
N	-1.261730000	3.949790000	-3.785404000	C	-4.438223000	-2.600620000	-2.653286000
N	-3.235576000	3.086677000	-3.383965000	C	-2.071942000	-3.477594000	-2.754620000
N	-4.388336000	0.697016000	-1.041597000	C	-1.918881000	-3.840915000	-5.028589000
N	-4.387564000	-0.701629000	-1.041512000	C	-3.157788000	-3.296816000	-4.774200000
N	-3.232770000	-3.090568000	-3.383758000	C	3.919812000	-2.017406000	2.798224000
N	-1.257981000	-3.951382000	-3.785482000	C	3.281102000	-2.968606000	4.790541000
N	3.259482000	-3.071941000	3.387768000	C	3.972532000	-1.817077000	5.094488000
N	4.355118000	-1.236856000	3.867051000	C	5.157928000	0.002075000	3.749473000
N	4.353502000	1.239955000	3.867317000	C	3.917041000	2.020026000	2.798621000
N	3.255584000	3.073762000	3.388327000	C	3.277645000	2.970411000	4.791097000
N	0.722536000	-3.550800000	1.098144000	C	3.970508000	1.819692000	5.094855000
N	0.718197000	3.551446000	1.098455000	C	2.607859000	-4.177524000	2.623328000
N	1.253933000	3.959440000	-3.780300000	C	1.141604000	-3.947368000	2.346811000
N	3.230439000	3.101403000	-3.380882000	C	2.602948000	4.178894000	2.624080000
N	4.263318000	0.701194000	-1.046842000	C	1.136900000	3.947626000	2.347382000
N	4.264075000	-0.697191000	-1.046971000	C	2.088207000	3.533534000	-2.747722000
N	3.233543000	-3.097863000	-3.381495000	C	1.883838000	3.780436000	-5.030213000

C	3.124198000	3.236985000	-4.777503000	H	4.247467000	1.402522000	6.055147000
C	4.434577000	2.602099000	-2.651975000	H	3.150915000	-4.277702000	1.672757000
C	4.369776000	1.128487000	-2.346438000	H	2.743109000	-5.101149000	3.204094000
C	4.441953000	0.002328000	-3.197740000	H	2.737376000	5.102522000	3.205027000
C	4.370969000	-1.124093000	-2.346665000	H	3.145954000	4.279766000	1.673555000
C	4.437331000	-2.597532000	-2.652719000	H	1.430037000	4.080479000	-5.966727000
C	2.091971000	-3.531530000	-2.748161000	H	3.929785000	2.979986000	-5.454260000
C	1.886967000	-3.777311000	-5.030685000	H	5.312168000	2.836994000	-3.271428000
C	3.126871000	-3.232730000	-4.778145000	H	4.504093000	3.166026000	-1.710605000
C	0.007285000	-4.183383000	3.157053000	H	4.561471000	0.002520000	-4.275939000
C	0.002369000	4.182596000	3.157656000	H	4.507730000	-3.161758000	-1.711595000
C	-0.007695000	4.712513000	-3.586654000	H	5.315023000	-2.831239000	-3.272480000
C	-0.002905000	-4.712366000	-3.586736000	H	1.433112000	-4.077241000	-5.967206000
H	-2.774469000	-3.691781000	5.413971000	H	3.931912000	-2.974510000	-5.455084000
H	-4.201698000	-1.395770000	6.056603000	H	-0.001522000	-4.540692000	4.181849000
H	-5.898926000	-0.003303000	4.589011000	H	-0.006704000	4.539384000	4.182629000
H	-5.687024000	-0.003161000	2.805107000	H	-0.011107000	5.111006000	-2.566601000
H	-2.779093000	3.689034000	5.414144000	H	-0.010002000	5.544018000	-4.304793000
H	-4.203594000	1.391272000	6.056635000	H	-0.005640000	-5.110695000	-2.566618000
H	-3.116732000	-4.224630000	1.633731000	H	-0.004203000	-5.544013000	-4.304712000
H	-2.730288000	-5.080694000	3.152971000	H	-3.982837000	3.073533000	-5.444292000
H	-2.736175000	5.078040000	3.153418000	C	-1.290432000	0.001140000	-0.808281000
H	-3.121698000	4.221780000	1.634039000	C	0.062058000	0.000437000	-0.701216000
H	-1.486641000	4.180137000	-5.959478000	H	-1.797255000	0.003144000	-1.774621000
H	-5.316212000	2.836124000	-3.274556000	H	-1.912091000	0.000869000	0.085625000
H	-4.510669000	3.162079000	-1.713703000	C	0.739068000	-0.000401000	0.656842000
H	-4.424361000	-0.002571000	-4.284410000	C	0.973480000	0.001075000	-1.915393000
H	-4.507478000	-3.166858000	-1.713193000	H	1.380266000	-0.891422000	0.766086000
H	-5.313616000	-2.841949000	-3.273956000	H	1.377424000	0.892450000	0.768218000
H	-1.484037000	-4.184699000	-5.959119000	H	-0.002178000	-0.002538000	1.472115000
H	-3.981434000	-3.080946000	-5.443594000	H	1.638476000	0.878625000	-1.901807000
H	2.848251000	-3.719493000	5.439609000	H	1.637824000	-0.876996000	-1.903417000
H	4.248780000	-1.399600000	6.054852000	H	0.398623000	0.002173000	-2.855729000
H	5.905350000	0.002485000	4.554165000	<u>C₄H₁₀@PPX</u>			
H	5.658587000	0.002512000	2.775208000	Au	4.084966000	-1.341087000	-0.805159000
H	2.844062000	3.720770000	5.440282000	Au	3.884161000	1.786449000	-0.804955000

Au	1.334167000	3.661154000	0.858769000	C	3.846037000	2.061269000	-5.048445000
Au	1.796342000	-3.497352000	0.860041000	C	2.876552000	-4.069299000	-2.586891000
Au	-3.867085000	-1.786443000	-0.866008000	C	1.398477000	-3.951418000	-2.310749000
Au	-4.070762000	1.333217000	-0.874113000	C	2.357345000	4.351446000	-2.582514000
Au	-1.808791000	3.483174000	0.827631000	C	0.900805000	4.064502000	-2.314262000
Au	-1.346503000	-3.635206000	0.837429000	C	1.792696000	3.697085000	2.812257000
N	3.434978000	-2.915425000	-3.351078000	C	1.594540000	3.946493000	5.094938000
N	4.372355000	-0.992315000	-3.816800000	C	2.848359000	3.437940000	4.836345000
N	4.223196000	1.485595000	-3.816894000	C	4.163201000	2.835525000	2.703305000
N	3.052188000	3.275883000	-3.348830000	C	4.146710000	1.361346000	2.396404000
N	0.946464000	-3.635476000	-1.052450000	C	4.316097000	0.243902000	3.245479000
N	0.479336000	3.708581000	-1.055796000	C	4.298598000	-0.885897000	2.396153000
N	0.952611000	4.102932000	3.847890000	C	4.510447000	-2.345002000	2.703338000
N	2.949619000	3.299448000	3.439875000	C	2.259832000	-3.482896000	2.812714000
N	4.029940000	0.925835000	1.100036000	C	2.094730000	-3.756967000	5.095417000
N	4.123553000	-0.469760000	1.099856000	C	3.284003000	-3.112031000	4.835758000
N	3.366349000	-2.960285000	3.439580000	C	-3.672770000	-2.237561000	-2.811625000
N	1.471617000	-3.980143000	3.849101000	C	-3.032236000	-3.198225000	-4.798409000
N	-2.988245000	-3.278801000	-3.394663000	C	-3.766677000	-2.075173000	-5.108985000
N	-4.151698000	-1.489638000	-3.884583000	C	-5.026230000	-0.300712000	-3.769244000
N	-4.308648000	0.988160000	-3.890875000	C	-3.927563000	1.794741000	-2.821461000
N	-3.376530000	2.909986000	-3.409403000	C	-3.408332000	2.817583000	-4.812812000
N	-0.452923000	-3.702510000	-1.061802000	C	-3.997150000	1.610375000	-5.118039000
N	-0.919542000	3.629639000	-1.069823000	C	-2.305838000	-4.352537000	-2.615426000
N	-1.549713000	3.967512000	3.821430000	C	-0.854048000	-4.064996000	-2.325404000
N	-3.436703000	2.948829000	3.374341000	C	-2.824679000	4.060513000	-2.635579000
N	-4.181642000	0.465222000	1.026835000	C	-1.351033000	3.938636000	-2.337686000
N	-4.082628000	-0.929254000	1.031498000	C	-2.317748000	3.471577000	2.769252000
N	-3.019871000	-3.292119000	3.387872000	C	-2.195966000	3.741405000	5.055528000
N	-1.031563000	-4.098613000	3.829610000	C	-3.380090000	3.097282000	4.772418000
C	3.986785000	-1.805684000	-2.754409000	C	-4.574184000	2.346431000	2.617499000
C	3.468979000	-2.812581000	-4.753740000	C	-4.375626000	0.884193000	2.319033000
C	4.061169000	-1.604677000	-5.049021000	C	-4.403207000	-0.243917000	3.170266000
C	5.092519000	0.294437000	-3.685630000	C	-4.216285000	-1.362569000	2.326297000
C	3.734758000	2.240547000	-2.753530000	C	-4.224109000	-2.836490000	2.631758000
C	3.106891000	3.184947000	-4.751600000	C	-1.849024000	-3.680831000	2.780338000

C	-1.699640000	-3.955150000	5.064511000	H	-5.483807000	2.504193000	3.214800000
C	-2.947985000	-3.444855000	4.784770000	H	-4.671561000	2.900700000	1.672959000
C	0.288366000	-4.221991000	-3.143601000	H	-4.568650000	-0.252348000	4.242384000
C	-0.228279000	4.210629000	-3.152898000	H	-4.253023000	-3.402641000	1.689554000
C	-0.338393000	4.803573000	3.660982000	H	-5.105681000	-3.105650000	3.231339000
C	0.258223000	-4.807375000	3.663884000	H	-1.261935000	-4.254263000	6.008987000
H	3.115730000	-3.599788000	-5.408002000	H	-3.778529000	-3.220184000	5.442502000
H	4.315507000	-1.165610000	-6.005785000	H	0.310836000	-4.533298000	-4.182910000
H	5.853808000	0.340252000	-4.475950000	H	-0.235052000	4.515966000	-4.194181000
H	5.574225000	0.323803000	-2.702262000	H	-0.350412000	5.230985000	2.652680000
H	2.662689000	3.925581000	-5.404778000	H	-0.390000000	5.611116000	4.403866000
H	4.157952000	1.661604000	-6.005491000	H	0.286195000	-5.232595000	2.654951000
H	3.423560000	-4.125919000	-1.635093000	H	0.290254000	-5.617331000	4.405233000
H	3.083931000	-4.979702000	-3.167430000	H	3.664450000	3.205615000	5.509308000
H	2.460637000	5.282860000	-3.157791000	H	1.900195000	0.050936000	-2.341996000
H	2.890127000	4.467066000	-1.627897000	C	0.855738000	-0.051258000	-2.003479000
H	1.137469000	4.236334000	6.033083000	C	0.766122000	0.045154000	-0.463799000
H	5.036430000	3.095349000	3.318966000	C	-0.687273000	0.005151000	0.059334000
H	4.213702000	3.403165000	1.762917000	C	-0.730932000	0.086249000	1.602692000
H	4.466903000	0.254009000	4.319772000	H	0.258352000	0.750524000	-2.474393000
H	4.635872000	-2.901259000	1.763220000	H	0.471383000	-1.025346000	-2.352998000
H	5.409606000	-2.487326000	3.319987000	H	1.232637000	0.984010000	-0.122463000
H	1.673821000	-4.097354000	6.033553000	H	1.343403000	-0.774062000	-0.001751000
H	4.070449000	-2.791271000	5.507680000	H	-1.179368000	-0.921160000	-0.285213000
H	-2.583710000	-3.943957000	-5.442788000	H	-1.248544000	0.849297000	-0.379046000
H	-4.069223000	-1.680780000	-6.071257000	H	-0.204317000	0.998533000	1.942505000
H	-5.775204000	-0.350115000	-4.570956000	H	-0.227562000	-0.796061000	2.040635000
H	-5.523324000	-0.329861000	-2.793565000	H	-1.763354000	0.125090000	1.979394000
H	-3.054693000	3.609914000	-5.460689000	<u>Iso-butane@PPX</u>			
H	-4.247275000	1.176789000	-6.078470000	Au	4.315802000	-1.067973000	-0.837608000
H	-2.853284000	-4.466387000	-1.668906000	Au	3.815198000	2.136020000	-0.838366000
H	-2.399981000	-5.285263000	-3.190034000	Au	1.044110000	3.789295000	0.808171000
H	-3.020850000	4.972404000	-3.217612000	Au	2.171028000	-3.414886000	0.829778000
H	-3.384897000	4.118168000	-1.691542000	Au	-3.863799000	-2.173116000	-0.801830000
H	-1.792948000	4.080462000	6.001960000	Au	-4.315595000	1.050860000	-0.824126000
H	-4.179513000	2.776132000	5.428683000	Au	-2.182005000	3.458808000	0.823123000

Au	-1.051378000	-3.743363000	0.846607000	C	1.530775000	3.790838000	2.759051000
N	3.616016000	-2.690934000	-3.368053000	C	1.321519000	3.961360000	5.049683000
N	4.351303000	-0.684657000	-3.849421000	C	2.610064000	3.560983000	4.775423000
N	3.968481000	1.768073000	-3.851287000	C	3.977212000	3.156404000	2.636076000
N	2.670077000	3.466311000	-3.373845000	C	4.153001000	1.690750000	2.332688000
N	1.265641000	-3.703949000	-1.043418000	C	4.373928000	0.587297000	3.188521000
N	0.096985000	3.864777000	-1.063759000	C	4.535896000	-0.527742000	2.335893000
N	0.663656000	4.101276000	3.808805000	C	4.810388000	-1.975780000	2.652990000
N	2.718045000	3.468682000	3.375514000	C	2.631019000	-3.256145000	2.778239000
N	4.186950000	1.263823000	1.029787000	C	2.429112000	-3.396731000	5.071386000
N	4.429212000	-0.116503000	1.030549000	C	3.580861000	-2.694738000	4.794111000
N	3.687383000	-2.625029000	3.392733000	C	-3.538876000	-2.568966000	-2.744225000
N	1.848688000	-3.735555000	3.830156000	C	-2.698253000	-3.368174000	-4.729380000
N	-2.720086000	-3.509447000	-3.329699000	C	-3.522232000	-2.308788000	-5.036065000
N	-4.028554000	-1.819097000	-3.813892000	C	-5.011110000	-0.713707000	-3.711165000
N	-4.410440000	0.635339000	-3.833866000	C	-4.142579000	1.502739000	-2.774354000
N	-3.662880000	2.643527000	-3.378047000	C	-3.633968000	2.509775000	-4.778237000
N	-0.126918000	-3.859259000	-1.035405000	C	-4.106918000	1.249509000	-5.067233000
N	-1.292147000	3.689859000	-1.063357000	C	-1.971311000	-4.555410000	-2.571404000
N	-1.829229000	3.807158000	3.820331000	C	-0.525920000	-4.205995000	-2.303720000
N	-3.655983000	2.670162000	3.402304000	C	-3.231106000	3.862398000	-2.631447000
N	-4.372902000	0.122666000	1.058535000	C	-1.749164000	3.897299000	-2.341992000
N	-4.170687000	-1.263796000	1.068619000	C	-2.613144000	3.312927000	2.777489000
N	-2.712705000	-3.453209000	3.426413000	C	-2.397290000	3.469501000	5.067448000
N	-0.645372000	-4.052829000	3.844897000	C	-3.542072000	2.750926000	4.802202000
C	4.101046000	-1.544252000	-2.779952000	C	-4.765334000	1.993128000	2.668262000
C	3.564913000	-2.566877000	-4.768335000	C	-4.470594000	0.546452000	2.360606000
C	4.030259000	-1.307687000	-5.073365000	C	-4.326796000	-0.564362000	3.223159000
C	4.952462000	0.666003000	-3.747411000	C	-4.136993000	-1.679598000	2.375998000
C	3.484146000	2.525249000	-2.784498000	C	-3.977722000	-3.143127000	2.695337000
C	2.642449000	3.316820000	-4.772554000	C	-1.522980000	-3.748807000	2.801561000
C	3.460495000	2.252109000	-5.075214000	C	-1.300304000	-3.935796000	5.089905000
C	3.197104000	-3.907735000	-2.610879000	C	-2.596872000	-3.555559000	4.824905000
C	1.716312000	-3.945015000	-2.317437000	C	0.612521000	-4.266847000	-3.143135000
C	1.933383000	4.522763000	-2.620161000	C	-0.650848000	4.209342000	-3.178523000
C	0.489396000	4.181081000	-2.341442000	C	-0.675318000	4.721030000	3.654479000

C	0.698749000	-4.657762000	3.679032000	H	-0.818506000	-4.165147000	6.032375000
H	3.249188000	-3.375162000	-5.415983000	H	-3.432034000	-3.392541000	5.494838000
H	4.193182000	-0.835952000	-6.034375000	H	0.639355000	-4.547916000	-4.190906000
H	5.673344000	0.776687000	-4.568917000	H	-0.683850000	4.464295000	-4.232726000
H	5.471616000	0.748843000	-2.786750000	H	-0.732856000	5.167720000	2.656312000
H	2.092267000	3.986316000	-5.421652000	H	-0.763008000	5.509449000	4.414611000
H	3.746923000	1.841341000	-6.035324000	H	0.750223000	-5.107616000	2.682153000
H	3.761684000	-3.913608000	-1.667487000	H	0.801254000	-5.443151000	4.440392000
H	3.495708000	-4.783521000	-3.204996000	H	3.445474000	3.379029000	5.440115000
H	1.999649000	5.450356000	-3.207458000	C	1.034162000	-0.145570000	1.106860000
H	2.464397000	4.670539000	-1.669105000	C	0.286301000	-0.410085000	-0.219114000
H	0.847965000	4.190922000	5.996252000	H	0.397135000	-1.471645000	-0.472372000
H	4.811594000	3.530702000	3.247504000	H	0.605992000	-0.767468000	1.914509000
H	3.952956000	3.723519000	1.694627000	H	2.096866000	-0.394640000	1.011768000
H	4.440134000	0.599623000	4.271164000	H	0.946931000	0.917944000	1.392319000
H	4.959575000	-2.536828000	1.719462000	C	0.856100000	0.416487000	-1.395788000
H	5.712410000	-2.080186000	3.273663000	C	-1.212174000	-0.123303000	-0.039840000
H	2.011307000	-3.706182000	6.021470000	H	0.222979000	0.299161000	-2.294839000
H	4.332068000	-2.286557000	5.458863000	H	0.890356000	1.485285000	-1.135088000
H	-2.146328000	-4.038218000	-5.376500000	H	1.877004000	0.091656000	-1.648500000
H	-3.811947000	-1.904579000	-5.998002000	H	-1.375747000	0.917485000	0.280508000
H	-5.741745000	-0.833444000	-4.522805000	H	-1.745280000	-0.269257000	-0.993562000
H	-5.517872000	-0.784944000	-2.742959000	H	-1.657860000	-0.789402000	0.714886000
H	-3.326449000	3.312506000	-5.436707000	<u>2C₂H₂@PPX</u>			
H	-4.286060000	0.771986000	-6.022528000	Au	4.095251000	0.997908000	0.831890000
H	-2.495498000	-4.701319000	-1.616077000	Au	3.616530000	-2.094813000	0.829147000
H	-2.034923000	-5.487807000	-3.151436000	Au	0.997029000	-3.803723000	-0.851740000
H	-3.525774000	4.735754000	-3.231258000	Au	2.110697000	3.403992000	-0.850432000
H	-3.792690000	3.880608000	-1.686376000	Au	-3.616559000	2.095059000	0.828765000
H	-1.977355000	3.790515000	6.012764000	Au	-4.094910000	-0.997763000	0.831845000
H	-4.283375000	2.337232000	5.474628000	Au	-2.110735000	-3.404352000	-0.850198000
H	-5.669702000	2.084542000	3.287745000	Au	-0.997098000	3.803538000	-0.852170000
H	-4.926303000	2.543966000	1.730596000	N	3.645607000	2.634669000	3.381211000
H	-4.387237000	-0.566004000	4.306225000	N	4.377581000	0.623496000	3.844265000
H	-3.968141000	-3.722758000	1.761194000	N	4.000731000	-1.833219000	3.841508000
H	-4.808415000	-3.501490000	3.320915000	N	2.700890000	-3.532533000	3.373017000

N	1.261866000	3.598983000	1.056112000	C	4.277850000	-0.609051000	-3.210438000
N	0.124637000	-3.784910000	1.055265000	C	4.328807000	0.523538000	-2.367586000
N	0.624289000	-4.239365000	-3.843518000	C	4.690593000	1.954859000	-2.671430000
N	2.662469000	-3.562733000	-3.415291000	C	2.583101000	3.335569000	-2.800294000
N	3.854885000	-1.253855000	-1.076150000	C	2.449649000	3.595318000	-5.086242000
N	4.069659000	0.131053000	-1.075367000	C	3.561579000	2.828106000	-4.816962000
N	3.626126000	2.685966000	-3.418641000	C	-3.444157000	2.541175000	2.778078000
N	1.854109000	3.900365000	-3.843973000	C	-2.781484000	3.460959000	4.774663000
N	-2.701244000	3.532992000	3.372542000	C	-3.601581000	2.394829000	5.072301000
N	-4.001127000	1.833744000	3.841114000	C	-4.972123000	0.725425000	3.705050000
N	-4.377692000	-0.623000000	3.844113000	C	-4.055905000	-1.466652000	2.783478000
N	-3.645754000	-2.634240000	3.381357000	C	-3.702666000	-2.538548000	4.783088000
N	-0.124887000	3.784843000	1.054889000	C	-4.166279000	-1.274910000	5.076895000
N	-1.262130000	-3.599082000	1.056456000	C	-1.930888000	4.556379000	2.604954000
N	-1.853912000	-3.900842000	-3.843683000	C	-0.505804000	4.157756000	2.320684000
N	-3.625860000	-2.686289000	-3.418517000	C	-3.205002000	-3.838809000	2.615742000
N	-4.068864000	-0.131219000	-1.075569000	C	-1.726892000	-3.854997000	2.323820000
N	-3.854286000	1.253717000	-1.076494000	C	-2.582979000	-3.336019000	-2.800069000
N	-2.662411000	3.562347000	-3.415783000	C	-2.449280000	-3.595707000	-5.086016000
N	-0.624138000	4.238751000	-3.843957000	C	-3.561178000	-2.828411000	-4.816834000
C	4.055826000	1.466997000	2.783498000	C	-4.690368000	-1.955109000	-2.671407000
C	3.702493000	2.539175000	4.782938000	C	-4.328586000	-0.523767000	-2.367650000
C	4.166114000	1.275583000	5.076953000	C	-4.278059000	0.608799000	-3.210590000
C	4.971850000	-0.725007000	3.705397000	C	-3.980814000	1.703806000	-2.366166000
C	3.443775000	-2.540699000	2.778494000	C	-3.894465000	3.177500000	-2.668113000
C	2.781075000	-3.460386000	4.775133000	C	-1.475557000	3.884055000	-2.799269000
C	3.601163000	-2.394227000	5.072723000	C	-1.287893000	4.127373000	-5.084476000
C	3.204745000	3.839045000	2.615401000	C	-2.568274000	3.698987000	-4.813388000
C	1.726628000	3.855055000	2.323495000	C	0.636756000	4.205284000	3.151354000
C	1.930662000	-4.556078000	2.605506000	C	-0.637049000	-4.205106000	3.151776000
C	0.505554000	-4.157610000	2.321156000	C	-0.719091000	-4.836261000	-3.671863000
C	1.475578000	-3.884421000	-2.798823000	C	0.719227000	4.835712000	-3.672264000
C	1.288164000	-4.128244000	-5.083999000	H	3.449606000	3.364067000	5.437233000
C	2.568491000	-3.699715000	-4.812884000	H	4.390847000	0.817307000	6.032092000
C	3.894452000	-3.177736000	-2.667594000	H	5.733921000	-0.842476000	4.487409000
C	3.980828000	-1.704001000	-2.365856000	H	5.439148000	-0.795676000	2.717396000

H	2.291941000	-4.173009000	5.427370000	H	-0.828417000	-5.635217000	-4.417738000
H	3.950686000	-2.025877000	6.029329000	H	0.777326000	5.261375000	-2.664694000
H	3.766634000	3.848718000	1.670389000	H	0.828538000	5.634645000	-4.418167000
H	3.489954000	4.722589000	3.204110000	H	3.405151000	-3.522872000	-5.477358000
H	1.956915000	-5.487639000	3.188997000	C	0.592966000	0.165123000	-1.291976000
H	2.460370000	-4.721126000	1.656459000	C	-0.591495000	-0.166506000	-1.295298000
H	0.824108000	-4.391660000	-6.026462000	H	1.626507000	0.446316000	-1.233970000
H	4.756192000	-3.498006000	-3.270795000	H	-1.625279000	-0.447731000	-1.242509000
H	3.896787000	-3.742609000	-1.724450000	C	0.608853000	-0.072034000	2.241686000
H	4.465513000	-0.638782000	-4.278560000	C	-0.611660000	0.075693000	2.245330000
H	4.863335000	2.496329000	-1.730291000	H	1.672749000	-0.200084000	2.183740000
H	5.606970000	2.000559000	-3.277305000	H	-1.675832000	0.203493000	2.194305000
H	2.068756000	3.967471000	-6.029338000	<u>2C₂H₄@PPX</u>			
H	4.308892000	2.416091000	-5.483716000	Au	-3.706923000	-1.870026000	0.822092000
H	-2.292394000	4.173644000	5.426860000	Au	-4.006316000	1.228944000	0.833242000
H	-3.951191000	2.026611000	6.028918000	Au	-1.883730000	3.495147000	-0.846877000
H	-5.734253000	0.842880000	4.486992000	Au	-1.230414000	-3.760455000	-0.868380000
H	-5.439367000	0.795928000	2.717034000	Au	3.992944000	-1.224699000	0.838014000
H	-3.449857000	-3.363370000	5.437504000	Au	3.725817000	1.877590000	0.847520000
H	-4.391040000	-0.816523000	6.031965000	Au	1.227899000	3.737294000	-0.838355000
H	-2.460552000	4.721386000	1.655892000	Au	1.890266000	-3.503406000	-0.865158000
H	-1.957063000	5.487998000	3.188346000	N	-2.912091000	-3.386511000	3.363367000
H	-3.490280000	-4.722201000	3.204641000	N	-4.098016000	-1.607162000	3.834183000
H	-3.766911000	-3.848602000	1.670762000	N	-4.322972000	0.869449000	3.842805000
H	-2.068296000	-3.967849000	-6.029080000	N	-3.478576000	2.836353000	3.383180000
H	-4.308385000	-2.416324000	-5.483661000	N	-0.361746000	-3.795966000	1.039460000
H	-5.606686000	-2.000804000	-3.277363000	N	-1.039256000	3.645366000	1.066981000
H	-4.863182000	-2.496510000	-1.730256000	N	-1.602025000	4.005283000	-3.838658000
H	-4.466183000	0.638454000	-4.278634000	N	-3.444428000	2.898558000	-3.415353000
H	-3.896868000	3.742519000	-1.725069000	N	-4.032733000	0.374067000	-1.078289000
H	-4.756154000	3.497648000	-3.271440000	N	-3.901606000	-1.018339000	-1.081664000
H	-0.823732000	4.390535000	-6.026957000	N	-2.872710000	-3.392353000	-3.429127000
H	-3.404876000	3.522070000	-5.477906000	N	-0.874848000	-4.175083000	-3.865851000
H	0.674869000	4.493793000	4.196693000	N	3.459677000	-2.854948000	3.375483000
H	-0.675185000	-4.493523000	4.197142000	N	4.304170000	-0.892500000	3.851870000
H	-0.777293000	-5.261861000	-2.664273000	N	4.081983000	1.584149000	3.859831000

N	2.897608000	3.365143000	3.393411000	C	2.971464000	3.286348000	4.795667000
N	1.033331000	-3.686162000	1.040306000	C	3.719696000	2.168368000	5.091777000
N	0.357472000	3.751097000	1.070654000	C	2.959476000	-4.027926000	2.600012000
N	0.892372000	4.209686000	-3.831259000	C	1.482787000	-3.963651000	2.307955000
N	2.890197000	3.424320000	-3.395407000	C	2.197267000	4.434837000	2.624561000
N	3.932475000	1.041348000	-1.059208000	C	0.752828000	4.120255000	2.333303000
N	4.054791000	-0.351728000	-1.065186000	C	1.717633000	3.803863000	-2.784122000
N	3.455195000	-2.859868000	-3.421203000	C	1.557701000	4.072839000	-5.068283000
N	1.617856000	-3.966837000	-3.862216000	C	2.812451000	3.575931000	-4.792251000
C	-3.580351000	-2.341594000	2.769849000	C	4.095570000	2.967642000	-2.641108000
C	-2.999522000	-3.320096000	4.765816000	C	4.093202000	1.490568000	-2.346389000
C	-3.748275000	-2.202969000	5.064377000	C	4.320537000	0.383145000	-3.194855000
C	-4.997715000	-0.439133000	3.699934000	C	4.292732000	-0.754028000	-2.355519000
C	-3.954981000	1.694745000	2.783620000	C	4.560494000	-2.203846000	-2.663681000
C	-3.538768000	2.741481000	4.785341000	C	2.371819000	-3.447827000	-2.812112000
C	-4.073084000	1.505763000	5.077102000	C	2.237778000	-3.692143000	-5.099775000
C	-2.210360000	-4.453912000	2.591753000	C	3.391047000	-2.992484000	-4.820318000
C	-0.764006000	-4.141498000	2.306161000	C	0.374390000	-4.248470000	3.137762000
C	-2.971312000	4.012925000	2.617081000	C	-0.389017000	4.244703000	3.156467000
C	-1.493779000	3.945891000	2.328372000	C	-0.418400000	4.876891000	-3.661063000
C	-2.359262000	3.474025000	-2.796736000	C	0.435639000	-4.842999000	-3.700755000
C	-2.222849000	3.752194000	-5.080609000	H	-2.567739000	-4.070331000	5.416438000
C	-3.379130000	3.052716000	-4.812333000	H	-4.082277000	-1.819228000	6.020513000
C	-4.552147000	2.233310000	-2.666505000	H	-5.766554000	-0.512594000	4.480737000
C	-4.278849000	0.782927000	-2.365549000	H	-5.467286000	-0.479010000	2.711181000
C	-4.305338000	-0.349387000	-3.211211000	H	-3.239994000	3.549753000	5.441086000
C	-4.068641000	-1.460827000	-2.370435000	H	-4.324371000	1.059692000	6.031474000
C	-4.076374000	-2.936072000	-2.674317000	H	-2.751890000	-4.580690000	1.643523000
C	-1.706732000	-3.788369000	-2.817572000	H	-2.292973000	-5.384567000	3.171361000
C	-1.529716000	-4.009687000	-5.104726000	H	-3.206254000	4.912796000	3.203195000
C	-2.784919000	-3.514276000	-4.828059000	H	-3.529674000	4.051723000	1.670914000
C	3.930828000	-1.705636000	2.785440000	H	-1.825065000	4.110869000	-6.022022000
C	3.527055000	-2.775432000	4.778407000	H	-5.464470000	2.338505000	-3.270985000
C	4.061157000	-1.541961000	5.080214000	H	-4.687411000	2.782471000	-1.723703000
C	4.980633000	0.417484000	3.722416000	H	-4.507512000	-0.366001000	-4.277029000
C	3.573102000	2.326638000	2.797740000	H	-4.107002000	-3.502006000	-1.732176000

H	-4.958789000	-3.202053000	-3.273967000	C	-0.759516000	0.105309000	2.018038000
H	-1.079468000	-4.285190000	-6.050453000	H	0.778886000	-1.137789000	2.843695000
H	-3.609623000	-3.281260000	-5.490159000	H	-1.592912000	-0.369821000	2.545064000
H	3.234757000	-3.592038000	5.426776000	H	1.345388000	0.162553000	1.633293000
H	4.316467000	-1.105240000	6.037846000	H	-1.017836000	0.918492000	1.334771000
H	5.745172000	0.482583000	4.508208000	<u>2Allene@PPX</u>			
H	5.456834000	0.463156000	2.737046000	Au	4.145443000	1.652646000	0.839398000
H	2.530443000	4.029101000	5.448574000	Au	4.201939000	-1.497108000	0.860560000
H	4.044702000	1.776572000	6.047742000	Au	1.679088000	-3.396746000	-0.804252000
H	3.519844000	-4.057805000	1.654690000	Au	1.540760000	3.442001000	-0.833736000
H	3.197347000	-4.930947000	3.180209000	Au	-4.214082000	1.502070000	0.792155000
H	2.274580000	5.362829000	3.208984000	Au	-4.139234000	-1.635481000	0.792867000
H	2.742169000	4.568208000	1.679180000	Au	-1.513197000	-3.430897000	-0.840221000
H	1.113956000	4.366477000	-6.011671000	Au	-1.669190000	3.384057000	-0.857590000
H	3.642938000	3.359703000	-5.452835000	N	3.164974000	3.127288000	3.348746000
H	4.976841000	3.241956000	-3.238544000	N	4.307350000	1.332231000	3.862848000
H	4.121889000	3.527752000	-1.695439000	N	4.351687000	-1.137780000	3.878862000
H	4.517047000	0.404951000	-4.261600000	N	3.276370000	-2.979579000	3.385067000
H	4.688759000	-2.758436000	-1.723083000	N	0.620991000	3.534421000	1.050251000
H	5.476211000	-2.309349000	-3.263140000	N	0.762690000	-3.492162000	1.082728000
H	1.841522000	-4.038005000	-6.046595000	N	1.383783000	-3.921768000	-3.786304000
H	4.165516000	-2.622725000	-5.480799000	N	3.350607000	-3.048664000	-3.366853000
H	0.396746000	-4.540342000	4.182684000	N	4.376759000	-0.630510000	-1.037445000
H	-0.414831000	4.547582000	4.198073000	N	4.355065000	0.767956000	-1.047875000
H	-0.455960000	5.300839000	-2.651712000	N	3.205930000	3.094212000	-3.402835000
H	-0.482242000	5.683563000	-4.403842000	N	1.205002000	3.888436000	-3.820606000
H	0.470649000	-5.281921000	-2.697815000	N	-3.327101000	3.005760000	3.317172000
H	0.503391000	-5.638813000	-4.454859000	N	-4.409499000	1.166713000	3.809026000
H	-4.154393000	2.695622000	-5.478876000	N	-4.367104000	-1.304929000	3.810910000
C	0.727277000	0.138525000	-1.303159000	N	-3.217049000	-3.104016000	3.325022000
C	-0.622918000	0.052072000	-1.355033000	N	-0.780885000	3.509736000	1.042705000
H	1.316415000	-0.520511000	-0.659682000	N	-0.638915000	-3.514270000	1.067761000
H	-1.172161000	-0.683042000	-0.759504000	N	-1.135328000	-3.941617000	-3.814936000
H	1.287802000	0.878248000	-1.881631000	N	-3.132548000	-3.121525000	-3.435515000
H	-1.223407000	0.722954000	-1.977212000	N	-4.344971000	-0.768739000	-1.103415000
C	0.519575000	-0.307422000	2.178904000	N	-4.398568000	0.628964000	-1.100755000

N	-3.300737000	3.019473000	-3.440795000	C	-1.768409000	-3.803432000	-5.069622000
N	-1.318633000	3.867774000	-3.839198000	C	-3.021069000	-3.284682000	-4.829378000
C	3.879014000	2.096927000	2.780924000	C	-4.361182000	-2.667871000	-2.719197000
C	3.144305000	3.023401000	4.751123000	C	-4.360371000	-1.194581000	-2.406816000
C	3.865068000	1.896518000	5.077008000	C	-4.427474000	-0.068589000	-3.259492000
C	5.138683000	0.111000000	3.772573000	C	-4.443849000	1.056763000	-2.404475000
C	3.952943000	-1.930430000	2.805998000	C	-4.510345000	2.529304000	-2.714033000
C	3.249447000	-2.859383000	4.786088000	C	-2.151190000	3.432414000	-2.806991000
C	3.928131000	-1.703077000	5.099364000	C	-1.958103000	3.711823000	-5.088229000
C	2.497626000	4.208278000	2.566533000	C	-3.201065000	3.175081000	-4.836316000
C	1.035151000	3.952248000	2.293818000	C	-0.100823000	4.190834000	3.099744000
C	2.652005000	-4.094586000	2.614340000	C	0.051536000	-4.170687000	3.128972000
C	1.183449000	-3.893372000	2.329333000	C	0.127094000	-4.687739000	-3.604526000
C	2.197126000	-3.472675000	-2.745611000	C	-0.065036000	4.633706000	-3.642735000
C	2.037103000	-3.765111000	-5.027525000	H	2.665167000	3.758530000	5.385328000
C	3.270644000	-3.212705000	-4.762634000	H	4.125327000	1.487774000	6.045445000
C	4.546461000	-2.542182000	-2.627595000	H	5.865713000	0.129488000	4.595595000
C	4.476480000	-1.065888000	-2.334119000	H	5.662907000	0.114119000	2.810787000
C	4.523090000	0.054622000	-3.195241000	H	2.796350000	-3.603660000	5.428694000
C	4.437221000	1.186296000	-2.352965000	H	4.171700000	-1.273685000	6.063196000
C	4.433254000	2.658585000	-2.669176000	H	3.039688000	4.302121000	1.614820000
C	2.043057000	3.485501000	-2.779597000	H	2.616560000	5.143963000	3.131611000
C	1.852619000	3.729809000	-5.064368000	H	2.799336000	-5.017174000	3.193956000
C	3.107210000	3.227217000	-4.800479000	H	3.203566000	-4.183454000	1.667637000
C	-3.995693000	1.953565000	2.737032000	H	1.601937000	-4.085285000	-5.966234000
C	-3.316898000	2.893655000	4.718705000	H	5.430599000	-2.781813000	-3.235882000
C	-3.999916000	1.739391000	5.031108000	H	4.606111000	-3.099302000	-1.681545000
C	-5.196034000	-0.083112000	3.700869000	H	4.627919000	0.048237000	-4.274853000
C	-3.917943000	-2.075273000	2.741006000	H	4.475036000	3.231653000	-1.731747000
C	-3.220582000	-2.993456000	4.726586000	H	5.297823000	2.932868000	-3.290691000
C	-3.946079000	-1.864436000	5.035191000	H	1.398538000	4.015716000	-6.005165000
C	-2.691834000	4.112416000	2.543385000	H	3.927053000	2.997527000	-5.469885000
C	-1.219525000	3.911048000	2.281197000	H	-2.873146000	3.642453000	5.362678000
C	-2.536705000	-4.186393000	2.555524000	H	-4.259416000	1.318802000	5.994768000
C	-1.071248000	-3.930889000	2.303684000	H	-5.932463000	-0.095359000	4.515548000
C	-1.981052000	-3.510683000	-2.791750000	H	-5.709573000	-0.092609000	2.733332000

H	-2.754903000	-3.726858000	5.372783000	<u>2C₃H₄@PPX</u>			
H	-4.227188000	-1.454389000	5.997329000	Au	1.837106000	-3.213615000	0.806169000
H	-3.228338000	4.187640000	1.587048000	Au	-1.397641000	-3.304509000	0.804036000
H	-2.850034000	5.041663000	3.109523000	Au	-4.169534000	-1.797715000	-0.890983000
H	-2.664281000	-5.120724000	3.121039000	Au	4.382956000	-1.378888000	-0.859903000
H	-3.063568000	-4.281998000	1.595565000	Au	1.394972000	3.331715000	0.782463000
H	-1.306896000	-4.112188000	-5.999513000	Au	-1.835103000	3.217876000	0.758873000
H	-3.831560000	-3.061624000	-5.512306000	Au	-4.392206000	1.370868000	-0.925387000
H	-5.221602000	-2.933140000	-3.350866000	Au	4.160744000	1.772826000	-0.859173000
H	-4.425389000	-3.238028000	-1.781179000	N	3.485867000	-2.842854000	3.384508000
H	-4.481964000	-0.069577000	-4.342812000	N	1.492358000	-3.660279000	3.788564000
H	-4.582502000	3.096359000	-1.774825000	N	-1.041218000	-3.756484000	3.785184000
H	-5.384209000	2.764911000	-3.338605000	N	-3.097545000	-3.114341000	3.369297000
H	-1.507690000	4.021360000	-6.023306000	N	4.515389000	-0.491445000	1.034788000
H	-4.012160000	2.933759000	-5.512276000	N	-4.438575000	-0.907320000	0.996360000
H	-0.112681000	4.558178000	4.120858000	N	-4.272622000	-1.487613000	-3.917495000
H	0.046875000	-4.537293000	4.150441000	N	-3.043124000	-3.214093000	-3.366178000
H	0.119286000	-5.086445000	-2.584584000	N	-0.467802000	-3.459854000	-1.082510000
H	0.142660000	-5.519039000	-4.322775000	N	0.932344000	-3.399036000	-1.083163000
H	-0.076338000	5.045251000	-2.627998000	N	3.459574000	-2.892913000	-3.363373000
H	-0.066191000	5.456896000	-4.370548000	N	4.478112000	-1.024194000	-3.882236000
H	4.088157000	-2.967038000	-5.429230000	N	3.052361000	3.123372000	3.372028000
C	-1.274335000	-0.001326000	-1.177070000	N	0.997579000	3.787208000	3.757352000
C	-0.012720000	-0.060658000	-1.578020000	N	-1.534420000	3.726048000	3.736207000
H	-1.594203000	-0.402712000	-0.212761000	N	-3.520593000	2.896460000	3.317724000
C	1.251326000	-0.088475000	-1.973497000	N	4.402989000	0.907192000	1.035919000
H	1.940812000	0.708203000	-1.692994000	N	-4.541075000	0.491845000	0.980986000
H	1.659628000	-0.906300000	-2.568419000	N	-4.421048000	0.976337000	-3.942452000
H	-2.031660000	0.475430000	-1.797579000	N	-3.406589000	2.847588000	-3.426004000
C	-1.259016000	0.001293000	2.886260000	N	-0.908686000	3.394589000	-1.124718000
C	-0.128906000	0.005846000	2.190232000	N	0.491268000	3.449050000	-1.112934000
H	-1.281064000	0.015852000	3.980576000	N	3.092735000	3.175038000	-3.371351000
C	0.953666000	0.019539000	1.426644000	N	4.328398000	1.440758000	-3.884206000
H	1.372230000	0.963603000	1.069926000	C	2.332038000	-3.245547000	2.753925000
H	1.417686000	-0.906207000	1.079939000	C	3.377264000	-2.970148000	4.782094000
H	-2.217335000	-0.013403000	2.362206000	C	2.127763000	-3.488621000	5.037352000

C	0.256663000	-4.452793000	3.595904000	C	0.911021000	3.907072000	-2.342113000
C	-1.901732000	-3.394265000	2.745804000	C	2.367426000	4.221110000	-2.589300000
C	-2.996935000	-3.270205000	4.765128000	C	3.866542000	2.188135000	-2.802801000
C	-1.707641000	-3.676609000	5.027261000	C	3.852705000	1.977320000	-5.098785000
C	4.705548000	-2.377076000	2.657699000	C	3.073976000	3.065547000	-4.773609000
C	4.640981000	-0.908122000	2.337794000	C	4.621688000	0.219105000	3.188026000
C	-4.356544000	-2.783952000	2.633785000	C	-4.606202000	-0.192283000	3.144755000
C	-4.469553000	-1.319913000	2.304225000	C	-5.160109000	-0.303879000	-3.853032000
C	-3.830493000	-2.224882000	-2.821496000	C	5.214635000	0.257647000	-3.791262000
C	-3.768919000	-2.030682000	-5.117703000	H	4.187922000	-2.725195000	5.457223000
C	-2.994260000	-3.113943000	-4.768426000	H	1.670324000	-3.777529000	5.975541000
C	-2.329385000	-4.251388000	-2.564302000	H	0.284549000	-5.281512000	4.317024000
C	-0.875142000	-3.936016000	-2.305575000	H	0.271593000	-4.858190000	2.578992000
C	0.264112000	-4.176823000	-3.110263000	H	-3.836970000	-3.123392000	5.432969000
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C	2.855613000	-4.010060000	-2.575685000	H	4.773200000	-2.954617000	1.724637000
C	4.120783000	-1.824635000	-2.799923000	H	5.574771000	-2.613340000	3.287852000
C	4.052908000	-1.608122000	-5.093784000	H	-5.195553000	-3.116533000	3.261845000
C	3.410171000	-2.780832000	-4.764740000	H	-4.357997000	-3.369658000	1.703260000
C	1.872817000	3.421985000	2.731684000	H	-4.027965000	-1.641298000	-6.094440000
C	2.927177000	3.262771000	4.767287000	H	-2.414308000	-5.203087000	-3.108826000
C	1.639760000	3.684076000	5.011139000	H	-2.861808000	-4.347148000	-1.607313000
C	-0.283953000	4.502232000	3.549059000	H	0.280795000	-4.587207000	-4.114938000
C	-2.357143000	3.289720000	2.696892000	H	3.399327000	-4.065185000	-1.621940000
C	-3.436701000	3.057937000	4.713083000	H	3.031435000	-4.939734000	-3.135503000
C	-2.191441000	3.584155000	4.977521000	H	4.270819000	-1.177808000	-6.063408000
C	4.323688000	2.799432000	2.656274000	H	2.967977000	-3.540165000	-5.397299000
C	4.457415000	1.335602000	2.338041000	H	3.751674000	3.094035000	5.448952000
C	-4.720495000	2.398438000	2.579604000	H	1.157833000	3.951200000	5.943569000
C	-4.633479000	0.924759000	2.280371000	H	-0.311471000	5.337071000	4.263078000
C	-4.084768000	1.789724000	-2.863320000	H	-0.286570000	4.898781000	2.528547000
C	-3.963554000	1.540599000	-5.151396000	H	-4.260182000	2.832546000	5.379678000
C	-3.323554000	2.714887000	-4.823870000	H	-1.752214000	3.900730000	5.915608000
C	-2.817454000	3.973786000	-2.642626000	H	4.331462000	3.379594000	1.722273000
C	-1.342860000	3.810319000	-2.360329000	H	5.151811000	3.143393000	3.292589000
C	-0.220472000	4.134991000	-3.158622000	H	-5.602692000	2.631072000	3.193098000

H	-4.784057000	2.960528000	1.636739000	Au	2.818101000	2.946959000	0.878705000
H	-4.159521000	1.096662000	-6.119479000	Au	-0.309055000	3.709146000	0.831377000
H	-2.862732000	3.463077000	-5.456322000	Au	-3.315291000	2.643635000	-0.860766000
H	-2.992501000	4.898459000	-3.211348000	Au	4.512180000	0.298543000	-0.794239000
H	-3.370747000	4.033486000	-1.694719000	N	1.990943000	-3.768236000	3.425784000
H	-0.229090000	4.528509000	-4.170095000	N	-0.152123000	-3.964699000	3.850413000
H	2.890360000	4.328305000	-1.628295000	N	-2.576479000	-3.268779000	3.836249000
H	2.457164000	5.165780000	-3.144810000	N	-4.244976000	-1.921445000	3.377599000
H	4.131581000	1.580738000	-6.067206000	N	3.849900000	-1.900079000	1.084548000
H	2.554335000	3.771835000	-5.408742000	N	-4.449757000	0.615252000	1.002583000
H	4.709447000	0.225755000	4.268800000	N	-4.426854000	0.077324000	-3.893652000
H	-4.683691000	-0.186280000	4.226486000	N	-4.113719000	-2.027274000	-3.380365000
H	-5.709154000	-0.327472000	-2.905424000	N	-1.956815000	-3.328121000	-1.036760000
H	-5.862712000	-0.354995000	-4.695688000	N	-0.606077000	-3.693555000	-1.034557000
H	5.744458000	0.290857000	-2.833023000	N	1.994794000	-3.783371000	-3.332476000
H	5.933647000	0.300879000	-4.620287000	N	3.613934000	-2.385984000	-3.814668000
H	-2.459031000	-3.822925000	-5.387335000	N	4.154258000	1.967729000	3.463093000
C	-1.301555000	-0.022859000	-0.159196000	N	2.491230000	3.333908000	3.875259000
C	-0.194004000	-0.010709000	-0.689623000	N	0.061500000	3.991183000	3.835258000
H	-2.230261000	-0.023656000	0.359693000	N	-2.068456000	3.758548000	3.361983000
C	1.169465000	0.016043000	-1.223901000	N	4.363895000	-0.598715000	1.090316000
H	1.882265000	0.018803000	-0.384008000	N	-3.912687000	1.906170000	1.005219000
H	1.386101000	-0.872677000	-1.837214000	N	-3.532530000	2.389938000	-3.883944000
H	1.352234000	0.928641000	-1.813471000	N	-1.921225000	3.779274000	-3.363003000
C	1.292321000	-0.081170000	2.294674000	N	0.649342000	3.636574000	-1.039571000
C	0.159751000	0.039300000	2.755104000	N	2.007436000	3.293490000	-1.022174000
H	2.246934000	-0.214467000	1.840753000	N	4.218451000	2.026814000	-3.318826000
C	-1.221251000	0.179901000	3.237521000	N	4.541993000	-0.081578000	-3.810781000
H	-1.272329000	0.777979000	4.162595000	C	0.766875000	-3.851330000	2.804034000
H	-1.836445000	0.677729000	2.473396000	C	1.859202000	-3.813212000	4.826279000
H	-1.669130000	-0.805364000	3.436245000	C	0.514712000	-3.941166000	5.094857000
<u>2C₃H₆@PPX</u>				C	-1.576656000	-4.352222000	3.690217000
Au	0.306703000	-3.752892000	0.849860000	C	-3.264233000	-2.675825000	2.775732000
Au	-2.788200000	-2.878138000	0.835305000	C	-4.180675000	-2.022557000	4.780215000
Au	-4.552754000	-0.294075000	-0.879230000	C	-3.137215000	-2.872945000	5.070587000
Au	3.315946000	-2.641538000	-0.802978000	C	3.288186000	-3.726100000	2.687792000

C	3.758113000	-2.328303000	2.384227000	C	4.215580000	-1.302903000	3.242109000
C	-5.248110000	-1.109282000	2.620937000	C	-4.376589000	1.340322000	3.151718000
C	-4.723614000	0.266187000	2.300983000	C	-4.732366000	1.521058000	-3.808278000
C	-4.395971000	-0.804834000	-2.815938000	C	4.821484000	-1.529879000	-3.706418000
C	-4.175024000	-0.604677000	-5.102297000	H	2.710244000	-3.792172000	5.495715000
C	-3.973481000	-1.926581000	-4.776166000	H	-0.000726000	-4.055999000	6.040522000
C	-3.910895000	-3.282262000	-2.598539000	H	-1.796514000	-5.109379000	4.455344000
C	-2.455521000	-3.543419000	-2.297376000	H	-1.696948000	-4.794959000	2.695945000
C	-1.424517000	-4.051722000	-3.120166000	H	-4.886239000	-1.527069000	5.435647000
C	-0.280587000	-4.134171000	-2.295068000	H	-2.786864000	-3.247927000	6.024355000
C	1.088832000	-4.699307000	-2.573109000	H	3.147991000	-4.277394000	1.747117000
C	2.956088000	-2.992526000	-2.745562000	H	4.027225000	-4.261692000	3.301640000
C	3.052744000	-2.802093000	-5.040138000	H	-6.160640000	-1.061940000	3.232149000
C	2.034387000	-3.677318000	-4.734571000	H	-5.470505000	-1.645609000	1.687419000
C	3.212210000	2.748534000	2.835884000	H	-4.200882000	-0.118355000	-6.069437000
C	4.036768000	2.049102000	4.862940000	H	-4.338785000	-4.109705000	-3.182514000
C	2.994965000	2.911875000	5.124208000	H	-4.474953000	-3.182197000	-1.660518000
C	1.481117000	4.402578000	3.702559000	H	-1.504858000	-4.353275000	-4.159352000
C	-0.828721000	3.838202000	2.769425000	H	1.591276000	-4.934186000	-1.624176000
C	-1.970716000	3.836660000	4.763818000	H	1.002263000	-5.625079000	-3.160415000
C	-0.635434000	3.986302000	5.063081000	H	3.438681000	-2.486750000	-6.001629000
C	5.143338000	1.126014000	2.726030000	H	1.380303000	-4.246329000	-5.383212000
C	4.583583000	-0.233569000	2.394323000	H	4.708061000	1.533103000	5.538236000
C	-3.355798000	3.732187000	2.602743000	H	2.610799000	3.277435000	6.068525000
C	-3.862736000	2.346703000	2.302980000	H	1.672711000	5.167367000	4.467814000
C	-2.902266000	2.995428000	-2.797813000	H	1.616691000	4.840898000	2.708146000
C	-2.939770000	2.802068000	-5.095358000	H	-2.837905000	3.821069000	5.412338000
C	-1.925533000	3.672997000	-4.765822000	H	-0.145547000	4.128738000	6.018517000
C	-1.019565000	4.676563000	-2.582066000	H	5.404552000	1.654421000	1.798061000
C	0.344127000	4.098340000	-2.297561000	H	6.041863000	1.044219000	3.354357000
C	1.504945000	4.042233000	-3.104031000	H	-4.089955000	4.294106000	3.198762000
C	2.527260000	3.534288000	-2.270376000	H	-3.186897000	4.270709000	1.659389000
C	3.990054000	3.286218000	-2.549014000	H	-3.303759000	2.487208000	-6.065465000
C	4.466056000	0.804265000	-2.738544000	H	-1.254524000	4.240577000	-5.398178000
C	4.350674000	0.597999000	-5.031895000	H	-0.919290000	5.612131000	-3.151429000
C	4.143270000	1.922471000	-4.719804000	H	-1.529125000	4.897375000	-1.633755000

H	1.601606000	4.365582000	-4.135357000	Au	-2.177832000	-3.066323000	-1.156217000
H	4.541584000	3.197728000	-1.602338000	Au	-4.354296000	-0.949286000	0.641557000
H	4.418217000	4.113600000	-3.132557000	Au	3.746273000	-2.200688000	0.693529000
H	4.420492000	0.108486000	-5.995367000	N	3.810712000	2.803318000	-3.254047000
H	3.994809000	2.780791000	-5.363010000	N	2.012143000	4.004151000	-3.599904000
H	4.299344000	-1.340688000	4.322860000	N	-0.476098000	4.357495000	-3.598853000
H	-4.492089000	1.386755000	4.229157000	N	-2.561939000	3.781257000	-3.256743000
H	-5.247537000	1.716750000	-2.861578000	N	4.334326000	0.118493000	-1.055237000
H	-5.389134000	1.782989000	-4.648890000	N	-4.045649000	1.434904000	-1.088860000
H	5.302571000	-1.724959000	-2.741946000	N	-4.062145000	1.572896000	3.855693000
H	5.502158000	-1.806143000	-4.523054000	N	-2.649746000	3.209672000	3.502166000
H	-3.785701000	-2.785338000	-5.408182000	N	-0.051988000	3.483546000	1.247751000
C	-1.121196000	-0.226799000	-1.796829000	N	1.338754000	3.309526000	1.237518000
C	0.191216000	-0.538334000	-1.889081000	N	3.750147000	2.359691000	3.504770000
H	-1.807016000	-0.863654000	-1.243879000	N	4.461767000	0.326701000	3.894918000
H	-1.531552000	0.681161000	-2.248578000	N	2.682347000	-3.297774000	-3.643691000
C	1.232346000	0.330911000	-2.556721000	N	0.612095000	-3.822064000	-4.128112000
H	0.557025000	-1.447775000	-1.402080000	N	-1.870664000	-3.445510000	-4.157778000
H	1.890576000	-0.258834000	-3.215640000	N	-3.684925000	-2.301813000	-3.712905000
H	0.768971000	1.142172000	-3.141193000	N	4.075165000	-1.253971000	-1.144212000
H	1.870856000	0.795624000	-1.787593000	N	-4.302873000	0.064448000	-1.191961000
C	-1.328987000	0.198286000	1.645037000	N	-4.608119000	-0.837772000	3.675512000
C	-0.149263000	-0.415433000	1.890235000	N	-3.876819000	-2.800936000	3.038525000
H	-2.231054000	-0.071812000	2.188851000	N	-1.376107000	-3.387505000	0.757375000
H	-1.417254000	0.968289000	0.876232000	N	0.016213000	-3.558200000	0.779843000
C	1.136351000	-0.082695000	1.171729000	N	2.548596000	-3.650367000	3.108151000
H	-0.101429000	-1.207925000	2.647038000	N	3.956131000	-2.092864000	3.731180000
H	1.510875000	-0.955099000	0.616574000	C	2.726568000	3.342417000	-2.603133000
H	0.980216000	0.735547000	0.453935000	C	3.784109000	3.101405000	-4.629118000
H	1.926861000	0.209394000	1.882398000	C	2.655153000	3.860402000	-4.848164000
<u>2(1,2-butadiene)@PPX</u>				C	0.873018000	4.915085000	-3.347212000
Au	2.196949000	3.192805000	-0.676133000	C	-1.364051000	3.949578000	-2.602902000
Au	-0.918000000	3.646324000	-0.667693000	C	-2.440031000	4.054304000	-4.631588000
Au	-3.772569000	2.118757000	0.869509000	C	-1.130182000	4.420509000	-4.848374000
Au	4.340163000	0.867585000	0.900634000	C	4.884267000	2.042948000	-2.549037000
Au	0.938946000	-3.447991000	-1.115948000	C	4.526110000	0.597750000	-2.327076000

C	-3.834738000	3.440716000	-2.555140000	C	-4.271006000	0.930848000	-3.289117000
C	-4.024738000	1.961926000	-2.354583000	C	-5.116804000	0.552136000	3.658171000
C	-3.504633000	2.354132000	2.845317000	C	4.996446000	-1.040247000	3.711956000
C	-3.550867000	1.951529000	5.114401000	H	4.565772000	2.791612000	-5.311845000
C	-2.661263000	2.978172000	4.889511000	H	2.291726000	4.326909000	-5.755566000
C	-1.847131000	4.263802000	2.813831000	H	0.996434000	5.790068000	-3.999782000
C	-0.423595000	3.864460000	2.516616000	H	0.917747000	5.230005000	-2.299050000
C	0.727846000	3.931155000	3.333592000	H	-3.278120000	4.004628000	-5.315747000
C	1.814716000	3.587904000	2.496948000	H	-0.637307000	4.748977000	-5.755202000
C	3.296918000	3.585638000	2.783555000	H	5.051015000	2.530162000	-1.577455000
C	4.212883000	1.231057000	2.868649000	H	5.799421000	2.132388000	-3.151828000
C	4.154700000	0.898763000	5.145871000	H	-4.656695000	3.865034000	-3.150108000
C	3.704275000	2.176675000	4.898728000	H	-3.813354000	3.941687000	-1.576629000
C	1.458588000	-3.528525000	-3.058336000	H	-3.879209000	1.501050000	6.042784000
C	2.616028000	-3.422792000	-5.043855000	H	-1.859983000	5.156274000	3.455938000
C	1.315647000	-3.755516000	-5.350415000	H	-2.363707000	4.500468000	1.872679000
C	-0.747199000	-4.393716000	-3.993844000	H	0.773734000	4.229599000	4.375932000
C	-2.625453000	-2.931660000	-3.105524000	H	3.857390000	3.636917000	1.839267000
C	-3.604278000	-2.399403000	-5.114092000	H	3.565879000	4.452958000	3.403070000
C	-2.466003000	-3.122683000	-5.396428000	H	4.315537000	0.383362000	6.084567000
C	3.928875000	-3.050435000	-2.862832000	H	3.402021000	2.959730000	5.582730000
C	4.107760000	-1.609840000	-2.468453000	H	3.481385000	-3.305674000	-5.684549000
C	-4.786171000	-1.645007000	-2.948394000	H	0.858519000	-3.982650000	-6.305745000
C	-4.441198000	-0.243534000	-2.521856000	H	-0.854844000	-5.173568000	-4.759964000
C	-4.281125000	-1.581476000	2.544502000	H	-0.826761000	-4.844547000	-2.998839000
C	-4.423573000	-1.604400000	4.844788000	H	-4.358840000	-1.990647000	-5.774806000
C	-3.961929000	-2.837381000	4.441083000	H	-2.066208000	-3.454065000	-6.346940000
C	-3.377351000	-3.913413000	2.174974000	H	3.877840000	-3.671429000	-1.956756000
C	-1.886904000	-3.868704000	1.940949000	H	4.772635000	-3.394784000	-3.478308000
C	-0.824721000	-4.353088000	2.734571000	H	-5.679290000	-1.653161000	-3.589693000
C	0.349897000	-4.147994000	1.976713000	H	-4.984034000	-2.260005000	-2.058377000
C	1.763871000	-4.591396000	2.254865000	H	-4.665170000	-1.236396000	5.834189000
C	3.422515000	-2.714482000	2.606429000	H	-3.725309000	-3.721649000	5.018826000
C	3.409965000	-2.644600000	4.907167000	H	-3.658729000	-4.858671000	2.660141000
C	2.523473000	-3.621788000	4.513038000	H	-3.904226000	-3.838257000	1.213137000
C	4.390035000	-0.465720000	-3.247803000	H	-0.897745000	-4.822679000	3.709760000

H	2.309736000	-4.698050000	1.306816000	Au	-2.700704000	-2.964072000	0.783130000
H	1.755340000	-5.565112000	2.765495000	Au	0.324132000	-3.933986000	0.829272000
H	3.716650000	-2.336857000	5.899060000	Au	3.255944000	-2.609246000	-0.790670000
H	1.922972000	-4.303794000	5.101288000	Au	-4.356373000	-0.321396000	-0.952945000
H	4.511210000	-0.419556000	-4.324732000	N	-2.114705000	3.799554000	3.381868000
H	-4.352854000	1.027018000	-4.366516000	N	0.003586000	4.082242000	3.870867000
H	-5.597981000	0.735534000	2.691340000	N	2.419308000	3.412948000	3.911285000
H	-5.851737000	0.656425000	4.467631000	N	4.052285000	2.016561000	3.485056000
H	5.517605000	-1.083954000	2.749386000	N	-3.733423000	1.837045000	0.984862000
H	5.702391000	-1.243377000	4.528601000	N	4.215666000	-0.547024000	1.116283000
H	-2.079503000	3.567525000	5.586909000	N	4.528714000	-0.047832000	-3.785527000
C	-0.095184000	0.146383000	-0.702001000	N	4.147707000	2.055856000	-3.312537000
C	0.774078000	0.166796000	-1.707326000	N	1.931497000	3.361795000	-1.002530000
C	0.417240000	0.551957000	-3.139707000	N	0.580466000	3.738665000	-1.019107000
C	-0.930131000	0.140235000	0.325908000	N	-1.969457000	3.886495000	-3.382384000
H	0.993469000	1.440522000	-3.449856000	N	-3.534600000	2.453006000	-3.919562000
H	-0.656117000	0.783179000	-3.227198000	N	-4.205910000	-2.057889000	3.300744000
H	0.665691000	-0.269168000	-3.836981000	N	-2.595804000	-3.463351000	3.782490000
H	-1.063103000	1.030176000	0.944909000	N	-0.174439000	-4.121998000	3.823054000
H	1.815218000	-0.099587000	-1.501635000	N	1.960551000	-3.822327000	3.423852000
H	-1.473337000	-0.760488000	0.618582000	N	-4.216534000	0.524486000	0.959889000
C	0.195100000	-0.536488000	3.370116000	N	3.724626000	-1.857124000	1.108202000
C	-0.832207000	-1.042916000	4.044327000	N	3.680678000	-2.390981000	-3.798034000
C	-0.719006000	-1.811118000	5.359155000	N	2.100589000	-3.842177000	-3.358108000
C	1.190538000	-0.010449000	2.668882000	N	-0.528115000	-3.781844000	-1.078231000
H	-1.322347000	-1.328887000	6.148345000	N	-1.868487000	-3.373855000	-1.100252000
H	0.326231000	-1.859600000	5.699709000	N	-3.986823000	-1.996440000	-3.486244000
H	-1.098357000	-2.841364000	5.238187000	N	-4.348503000	0.108902000	-3.965075000
H	1.520236000	1.017365000	2.832586000	C	-0.875550000	3.920229000	2.798392000
H	-1.841029000	-0.898681000	3.637906000	C	-2.029117000	3.865183000	4.784247000
H	1.676978000	-0.557031000	1.856924000	C	-0.699532000	4.047178000	5.094101000
<u>2(1,3-butadiene)@PPX</u>				C	1.423507000	4.494043000	3.748235000
Au	-0.355294000	3.822798000	0.859829000	C	3.126860000	2.821144000	2.866190000
Au	2.730436000	3.031104000	0.910737000	C	3.936646000	2.086646000	4.885061000
Au	4.358608000	0.342734000	-0.775940000	C	2.913629000	2.968407000	5.156088000
Au	-3.268212000	2.649309000	-0.892550000	C	-3.388894000	3.698722000	2.606625000

C	-3.785679000	2.284674000	2.281120000	C	-4.304381000	1.260727000	3.104250000
C	5.029397000	1.164814000	2.743039000	C	4.146987000	-1.281322000	3.261287000
C	4.467789000	-0.194551000	2.417080000	C	4.845357000	-1.486592000	-3.654259000
C	4.354370000	0.831349000	-2.720777000	C	-4.698833000	1.541208000	-3.847021000
C	4.438047000	0.637087000	-5.014115000	H	-2.899724000	3.818889000	5.426686000
C	4.194991000	1.959670000	-4.715224000	H	-0.218888000	4.192608000	6.053781000
C	3.906943000	3.311542000	-2.541725000	H	1.616106000	5.248706000	4.522910000
C	2.445990000	3.563187000	-2.260681000	H	1.563372000	4.940878000	2.758410000
C	1.428645000	4.076522000	-3.097413000	H	4.596322000	1.548786000	5.554560000
C	0.276195000	4.179952000	-2.284833000	H	2.537614000	3.333172000	6.103968000
C	-1.077574000	4.775047000	-2.583305000	H	-3.249547000	4.263604000	1.673930000
C	-2.917746000	3.057310000	-2.827065000	H	-4.168291000	4.193868000	3.203781000
C	-2.967660000	2.911353000	-5.127053000	H	5.931995000	1.082117000	3.365465000
C	-1.981857000	3.810025000	-4.787312000	H	5.286816000	1.690060000	1.812147000
C	-3.210773000	-2.804505000	2.718126000	H	4.585930000	0.152210000	-5.971223000
C	-4.224410000	-2.228359000	4.696480000	H	4.334575000	4.142041000	-3.121381000
C	-3.215698000	-3.115430000	5.001870000	H	4.456236000	3.222996000	-1.593504000
C	-1.585412000	-4.538117000	3.645481000	H	1.523649000	4.370506000	-4.137453000
C	0.754201000	-3.998612000	2.789506000	H	-1.598214000	4.996109000	-1.640928000
C	1.805612000	-3.818522000	4.821919000	H	-0.959704000	5.712657000	-3.145834000
C	0.465463000	-4.010149000	5.075085000	H	-3.326433000	2.601412000	-6.100725000
C	-5.140652000	-1.187321000	2.524939000	H	-1.333984000	4.411171000	-5.412755000
C	-4.560433000	0.172633000	2.240917000	H	-4.954154000	-1.747210000	5.335961000
C	3.265680000	-3.719913000	2.703780000	H	-2.924781000	-3.543346000	5.953389000
C	3.683059000	-2.304364000	2.404705000	H	-1.807052000	-5.298999000	4.406201000
C	2.991582000	-2.990398000	-2.745301000	H	-1.686507000	-4.978325000	2.647737000
C	3.208051000	-2.869564000	-5.036686000	H	2.641479000	-3.720818000	5.503326000
C	2.213062000	-3.779964000	-4.759119000	H	-0.060453000	-4.109899000	6.016505000
C	1.185782000	-4.756593000	-2.613393000	H	-5.357646000	-1.699301000	1.576330000
C	-0.177723000	-4.171863000	-2.347249000	H	-6.070590000	-1.107312000	3.105803000
C	-1.294968000	-4.018628000	-3.199787000	H	4.018746000	-4.222303000	3.328516000
C	-2.337668000	-3.522576000	-2.383059000	H	3.163284000	-4.276856000	1.761665000
C	-3.785667000	-3.255083000	-2.712538000	H	3.630103000	-2.563325000	-5.985914000
C	-4.268750000	-0.784029000	-2.900782000	H	1.623469000	-4.399924000	-5.422896000
C	-4.122210000	-0.555537000	-5.188571000	H	1.096171000	-5.680035000	-3.203737000
C	-3.890873000	-1.878702000	-4.885136000	H	1.674010000	-4.997333000	-1.658413000

H	-1.355188000	-4.274240000	-4.252495000	Au	1.452052000	3.323183000	-0.812107000
H	-4.366218000	-3.165412000	-1.783354000	Au	-4.393296000	1.443755000	0.970764000
H	-4.199350000	-4.081056000	-3.309035000	Au	-4.221303000	-1.740288000	0.958482000
H	-4.181517000	-0.058201000	-6.148661000	Au	-1.461730000	-3.275768000	-0.759579000
H	-3.712084000	-2.726801000	-5.534153000	Au	-1.791945000	3.224356000	-0.750203000
H	-4.489130000	1.307075000	4.171941000	N	3.200021000	3.126246000	3.315291000
H	4.261816000	-1.330431000	4.338753000	N	4.454147000	1.401856000	3.813279000
H	5.293065000	-1.654884000	-2.668960000	N	4.561078000	-1.058327000	3.821913000
H	5.569900000	-1.746250000	-4.437886000	N	3.464726000	-2.890540000	3.336910000
H	-5.204244000	1.698019000	-2.887760000	N	0.565640000	3.435195000	1.091899000
H	-5.379060000	1.795168000	-4.671336000	N	0.888815000	-3.386591000	1.102615000
H	4.094209000	2.819454000	-5.365852000	N	1.366741000	-3.718944000	-3.769572000
C	0.469211000	0.316048000	2.106082000	N	3.370004000	-2.902324000	-3.409887000
C	-0.458946000	-0.500258000	2.892663000	N	4.544439000	-0.545813000	-1.094666000
C	-1.156486000	-0.048053000	3.972185000	N	4.466667000	0.857231000	-1.101574000
C	1.112581000	-0.167727000	1.010503000	N	3.060185000	3.078713000	-3.429267000
H	0.599177000	1.365450000	2.396991000	N	1.005846000	3.763433000	-3.782235000
H	-0.594689000	-1.533202000	2.548016000	N	-3.329142000	2.904704000	3.448955000
H	-1.043859000	0.981400000	4.327582000	N	-4.388785000	1.066169000	3.990300000
H	-1.845568000	-0.688056000	4.525715000	N	-4.279755000	-1.395608000	3.982836000
H	1.758969000	0.445379000	0.389283000	N	-3.064333000	-3.131753000	3.432147000
H	0.986660000	-1.200806000	0.687868000	N	-0.834520000	3.399261000	1.117746000
C	0.472736000	0.386448000	-2.880507000	N	-0.511653000	-3.425760000	1.117858000
C	-0.441774000	-0.346575000	-2.002568000	N	-1.164411000	-3.823267000	-3.733799000
C	-0.961278000	0.195947000	-0.866706000	N	-3.200604000	-3.131144000	-3.302673000
C	1.049184000	-0.148150000	-3.994200000	N	-4.488834000	-0.856696000	-0.933201000
H	0.696001000	1.420972000	-2.599612000	N	-4.567831000	0.544367000	-0.928113000
H	-0.673284000	-1.379016000	-2.276564000	N	-3.513893000	2.933092000	-3.291642000
H	-0.724895000	1.222374000	-0.579155000	N	-1.525801000	3.746871000	-3.731809000
H	-1.598133000	-0.367274000	-0.185805000	C	3.970282000	2.143103000	2.737625000
H	1.720947000	0.433157000	-4.628877000	C	3.200467000	3.017899000	4.717284000
H	0.839932000	-1.178810000	-4.298612000	C	3.990004000	1.935174000	5.033204000
<u>2(1-butyn)e)@PPX</u>				C	5.322143000	0.206948000	3.710431000
Au	4.240525000	1.720939000	0.792020000	C	4.147769000	-1.848751000	2.752144000
Au	4.388560000	-1.415953000	0.805707000	C	3.449897000	-2.769099000	4.737732000
Au	1.775964000	-3.261859000	-0.798049000	C	4.140687000	-1.618662000	5.045538000

C	2.468040000	4.174017000	2.543925000	C	-3.453700000	3.120096000	-4.685295000
C	1.005080000	3.875058000	2.319980000	C	-0.114350000	4.113316000	3.150098000
C	2.820843000	-4.001404000	2.574463000	C	0.233585000	-4.113702000	3.151095000
C	1.343557000	-3.805359000	2.332276000	C	0.136235000	-4.514298000	-3.548825000
C	2.232671000	-3.309546000	-2.753904000	C	-0.260734000	4.500612000	-3.556275000
C	1.972009000	-3.540473000	-5.032892000	H	2.686253000	3.722526000	5.358590000
C	3.227124000	-3.022464000	-4.805099000	H	4.284289000	1.541091000	5.997998000
C	4.608433000	-2.446505000	-2.710494000	H	6.055093000	0.241521000	4.527403000
C	4.577560000	-0.974308000	-2.398373000	H	5.836763000	0.226602000	2.743688000
C	4.532710000	0.146198000	-3.255491000	H	2.996436000	-3.509731000	5.384279000
C	4.450057000	1.273098000	-2.408183000	H	4.396025000	-1.191417000	6.007282000
C	4.337159000	2.737749000	-2.732834000	H	2.974203000	4.272136000	1.573238000
C	1.897905000	3.400917000	-2.769889000	H	2.576562000	5.120279000	3.093448000
C	1.622184000	3.636702000	-5.047152000	H	2.988604000	-4.928266000	3.141556000
C	2.909164000	3.202289000	-4.823352000	H	3.345485000	-4.079249000	1.611782000
C	-4.049106000	1.865969000	2.902219000	H	1.493288000	-3.826522000	-5.961309000
C	-3.224649000	2.773840000	4.845539000	H	5.461398000	-2.699883000	-3.356605000
C	-3.892754000	1.620019000	5.188683000	H	4.689286000	-3.019194000	-1.775381000
C	-5.152011000	-0.200753000	3.918416000	H	4.554411000	0.142501000	-4.339572000
C	-3.859734000	-2.148253000	2.888858000	H	4.370893000	3.322459000	-1.802216000
C	-2.989593000	-3.013551000	4.831764000	H	5.160244000	3.064280000	-3.385019000
C	-3.755492000	-1.924061000	5.180741000	H	1.125707000	3.898779000	-5.973335000
C	-2.718813000	4.009584000	2.652841000	H	3.717957000	3.015182000	-5.518930000
C	-1.249856000	3.812570000	2.360560000	H	-2.731398000	3.510610000	5.466824000
C	-2.364824000	-4.178184000	2.630920000	H	-4.084829000	1.185442000	6.161713000
C	-0.911474000	-3.874594000	2.353929000	H	-5.845895000	-0.234328000	4.769129000
C	-1.998431000	-3.410946000	-2.692288000	H	-5.711021000	-0.222854000	2.976610000
C	-1.856197000	-3.783452000	-4.964175000	H	-2.445795000	-3.716367000	5.450196000
C	-3.132054000	-3.344496000	-4.692435000	H	-3.996723000	-1.521739000	6.156738000
C	-4.436676000	-2.748210000	-2.555409000	H	-3.277644000	4.075345000	1.708514000
C	-4.502468000	-1.277409000	-2.239586000	H	-2.868209000	4.942795000	3.215159000
C	-4.601718000	-0.152404000	-3.089096000	H	-2.448870000	-5.125506000	3.183345000
C	-4.628223000	0.970188000	-2.231664000	H	-2.907706000	-4.278722000	1.680345000
C	-4.707365000	2.442930000	-2.539364000	H	-1.410460000	-4.098015000	-5.899797000
C	-2.336456000	3.305635000	-2.684274000	H	-3.982360000	-3.206502000	-5.348917000
C	-2.207761000	3.636161000	-4.962788000	H	-5.294612000	-3.059371000	-3.168914000

H	-4.448373000	-3.322540000	-1.617737000	Au	0.690309000	3.513909000	0.871336000
H	-4.667969000	-0.152945000	-4.171352000	Au	2.598311000	-3.154235000	0.818195000
H	-4.761173000	3.009934000	-1.598698000	Au	-3.816890000	-2.386819000	-0.857831000
H	-5.594437000	2.677006000	-3.145471000	Au	-4.730409000	0.713122000	-0.862651000
H	-1.779831000	3.959770000	-5.903598000	Au	-2.570798000	3.023500000	0.804704000
H	-4.290482000	2.912768000	-5.340971000	Au	-0.729482000	-3.435231000	0.764262000
H	-0.106799000	4.502276000	4.163366000	N	4.146413000	-2.226841000	-3.302926000
H	0.255729000	-4.507460000	4.162326000	N	4.900093000	-0.207962000	-3.701852000
H	0.165975000	-4.902790000	-2.525767000	N	4.200130000	2.157764000	-3.664165000
H	0.157838000	-5.354267000	-4.256912000	N	2.539179000	3.518978000	-3.219157000
H	-0.243423000	4.893454000	-2.534542000	N	1.691884000	-3.269812000	-1.069110000
H	-0.281815000	5.338479000	-4.266900000	N	-0.214861000	3.487442000	-1.022742000
H	4.021282000	-2.774656000	-5.498562000	N	0.164940000	3.835856000	3.849500000
C	-0.286085000	0.001731000	0.816635000	N	2.297406000	3.433823000	3.508632000
C	1.073623000	0.030761000	1.365441000	N	4.256876000	1.535467000	1.215841000
C	1.137078000	0.017241000	2.916393000	N	4.684579000	0.200126000	1.201087000
C	-1.379813000	-0.003416000	0.258966000	N	3.976828000	-2.407843000	3.470308000
H	2.187092000	0.064809000	3.240606000	N	2.127071000	-3.542980000	3.789205000
H	0.685296000	-0.905211000	3.315228000	N	-2.368113000	-3.409055000	-3.378276000
H	0.598996000	0.883859000	3.333382000	N	-3.991306000	-2.022503000	-3.871528000
H	-2.276500000	0.004738000	-0.311816000	N	-4.697568000	0.332467000	-3.878459000
H	1.568425000	0.938559000	0.983536000	N	-3.989936000	2.343074000	-3.377262000
H	1.626039000	-0.835008000	0.965361000	N	0.302683000	-3.452293000	-1.085432000
C	0.255382000	-0.037807000	-2.447705000	N	-1.600299000	3.282980000	-1.049550000
C	-1.115296000	-0.003950000	-2.979471000	N	-2.328917000	3.431818000	3.792177000
C	-1.181697000	-0.036866000	-4.532869000	N	-4.151101000	2.289143000	3.356946000
C	1.372673000	-0.062065000	-1.938027000	N	-4.723046000	-0.237086000	1.011800000
H	-2.231954000	-0.015133000	-4.865380000	N	-4.316880000	-1.573027000	1.011731000
H	-0.708438000	-0.952591000	-4.921538000	N	-2.493051000	-3.520863000	3.318317000
H	-0.657009000	0.831749000	-4.962363000	N	-0.372833000	-3.923627000	3.737240000
H	2.291914000	-0.114476000	-1.401705000	C	4.615435000	-1.098224000	-2.666452000
H	-1.615729000	0.899670000	-2.599278000	C	4.160671000	-2.067976000	-4.701702000
H	-1.672522000	-0.856236000	-2.560975000	C	4.636351000	-0.801938000	-4.955241000
<u>2(2-butynyl)@PPX</u>				C	5.329914000	1.201761000	-3.535854000
Au	4.746999000	-0.682301000	-0.707226000	C	3.513123000	2.757540000	-2.608425000
Au	3.823994000	2.384968000	-0.658302000	C	2.618912000	3.419676000	-4.621437000

C	3.661253000	2.566955000	-4.902923000	C	-1.053333000	-3.957270000	4.974404000
C	3.665967000	-3.451501000	-2.595077000	C	-2.379099000	-3.700680000	4.710163000
C	2.173078000	-3.478275000	-2.338235000	C	1.091167000	-3.821086000	-3.185948000
C	1.593810000	4.412989000	-2.485808000	C	-0.947327000	3.931391000	-3.125815000
C	0.186975000	3.890125000	-2.277100000	C	-1.202170000	4.381697000	3.635627000
C	1.106779000	3.611825000	2.838724000	C	0.998578000	-4.474622000	3.558196000
C	0.784104000	3.781746000	5.117716000	H	3.877015000	-2.860802000	-5.382556000
C	2.119369000	3.525839000	4.901722000	H	4.840508000	-0.305656000	-5.895744000
C	3.625562000	3.314537000	2.831954000	H	6.063213000	1.432420000	-4.320095000
C	4.037535000	1.898727000	2.519847000	H	5.784957000	1.321926000	-2.546914000
C	4.326627000	0.800913000	3.363156000	H	1.973506000	3.980865000	-5.285400000
C	4.719525000	-0.247551000	2.499388000	H	4.076976000	2.261128000	-5.854882000
C	5.096324000	-1.677705000	2.801061000	H	4.204675000	-3.499989000	-1.637881000
C	2.972260000	-3.055612000	2.789288000	H	3.959769000	-4.317270000	-3.206189000
C	2.625470000	-3.201486000	5.065195000	H	1.548115000	5.358633000	-3.046597000
C	3.782693000	-2.482655000	4.862161000	H	2.051217000	4.615360000	-1.507202000
C	-3.388980000	-2.684438000	-2.801111000	H	0.250134000	3.967214000	6.041562000
C	-2.332964000	-3.224135000	-4.772509000	H	4.362034000	3.798358000	3.490939000
C	-3.352952000	-2.354820000	-5.084808000	H	3.567632000	3.888687000	1.896014000
C	-5.134620000	-1.079929000	-3.781966000	H	4.283417000	0.775299000	4.446613000
C	-4.502100000	1.199812000	-2.803011000	H	5.327206000	-2.204483000	1.863995000
C	-3.887034000	2.214374000	-4.774405000	H	5.970679000	-1.734293000	3.465699000
C	-4.333748000	0.952270000	-5.092212000	H	2.154745000	-3.519778000	5.987069000
C	-1.461529000	-4.325526000	-2.628135000	H	4.484962000	-2.065286000	5.573306000
C	-0.063325000	-3.808787000	-2.364607000	H	-1.634136000	-3.745736000	-5.414149000
C	-3.535935000	3.540378000	-2.611260000	H	-3.693924000	-1.994299000	-6.047038000
C	-2.049607000	3.551194000	-2.319976000	H	-5.817023000	-1.288317000	-4.616919000
C	-3.097053000	2.925371000	2.739969000	H	-5.650154000	-1.233830000	-2.827882000
C	-2.915922000	3.104582000	5.033966000	H	-3.554433000	3.023609000	-5.412301000
C	-4.055263000	2.382281000	4.758470000	H	-4.462783000	0.478109000	-6.057009000
C	-5.255103000	1.587069000	2.627397000	H	-1.953821000	-4.543777000	-1.670275000
C	-4.901074000	0.154428000	2.314683000	H	-1.399471000	-5.260632000	-3.204946000
C	-4.626618000	-0.940518000	3.168826000	H	-3.812826000	4.429822000	-3.195704000
C	-4.240963000	-1.998416000	2.313309000	H	-4.098161000	3.552611000	-1.666727000
C	-3.804349000	-3.410765000	2.598742000	H	-2.513355000	3.437215000	5.982809000
C	-1.267698000	-3.638636000	2.695975000	H	-4.806756000	1.974738000	5.423516000

H	-6.154250000	1.654565000	3.256579000	Au	-4.463536000	0.045947000	-0.948795000
H	-5.433512000	2.136579000	1.691887000	Au	-3.073554000	-2.754730000	0.757651000
H	-4.694262000	-0.961352000	4.251154000	Au	0.007362000	3.722048000	0.876951000
H	-3.697414000	-3.956315000	1.650200000	Au	4.547152000	-0.040625000	-0.787313000
H	-4.546201000	-3.934692000	3.219286000	Au	3.062514000	-2.831280000	-0.800504000
H	-0.563274000	-4.200400000	5.909171000	Au	-0.054563000	-3.811877000	0.803780000
H	-3.234792000	-3.674588000	5.373650000	Au	3.050110000	2.725321000	0.912784000
H	1.146129000	-4.103142000	-4.232692000	N	-1.588041000	4.000038000	-3.332057000
H	-0.976584000	4.251947000	-4.162521000	N	-3.287346000	2.733216000	-3.885739000
H	-1.246258000	4.801471000	2.625331000	N	-4.356966000	0.492078000	-3.954753000
H	-1.345752000	5.186067000	4.370419000	N	-4.227946000	-1.645131000	-3.495673000
H	1.078653000	-4.858371000	2.536125000	N	0.947774000	3.594664000	-1.000720000
H	1.104053000	-5.306049000	4.269056000	N	-2.242182000	-3.171411000	-1.122841000
H	2.941244000	3.446011000	5.602583000	N	-2.944663000	-3.229860000	3.760352000
C	-1.508677000	-0.072957000	-0.454204000	N	-4.454054000	-1.713441000	3.294107000
C	-1.536789000	-0.053727000	0.774770000	N	-4.250570000	0.878065000	0.966442000
C	-1.432720000	0.031844000	2.240484000	N	-3.621557000	2.127555000	1.002958000
C	-1.456548000	-0.091299000	-1.922085000	N	-1.736582000	3.848146000	3.411290000
H	-0.766540000	0.865847000	2.519985000	N	0.402708000	3.948460000	3.883855000
H	-1.022436000	-0.900672000	2.663315000	N	4.397797000	1.705708000	-3.307289000
H	-0.842695000	-0.937437000	-2.263903000	N	4.588696000	-0.420228000	-3.798957000
H	-1.009359000	0.841147000	-2.295493000	N	3.478240000	-2.646603000	-3.809811000
H	-2.408726000	0.219940000	2.701540000	N	1.732168000	-3.892253000	-3.361625000
H	-2.456188000	-0.199442000	-2.360071000	N	2.264754000	3.114666000	-0.995231000
C	1.566559000	0.104986000	-1.769499000	N	-0.919858000	-3.631688000	-1.098889000
C	1.522847000	0.042447000	-0.542508000	N	-0.557112000	-4.007530000	3.795479000
C	1.482250000	-0.069508000	0.918418000	N	1.596063000	-3.874813000	3.396344000
C	1.494875000	0.168875000	-3.237525000	N	3.653757000	-2.154993000	1.090501000
H	2.471715000	-0.289964000	1.326680000	N	4.313089000	-0.921372000	1.102326000
H	0.808196000	-0.888685000	1.207906000	N	4.326076000	1.642325000	3.486108000
H	1.012581000	-0.735887000	-3.645198000	N	2.777053000	3.130964000	3.913626000
H	2.487761000	0.248095000	-3.695993000	C	-2.625555000	3.277518000	-2.786963000
H	1.115599000	0.853701000	1.386008000	C	-1.589296000	3.916709000	-4.736577000
H	0.909485000	1.044724000	-3.565386000	C	-2.658437000	3.123578000	-5.086748000
<u>2C₄H₈@PPX</u>				C	-4.546147000	1.953949000	-3.827410000
Au	-3.042555000	2.904249000	-0.858565000	C	-4.395432000	-0.415756000	-2.899703000

C	-4.089835000	-1.522567000	-4.890946000	C	3.444012000	2.495069000	2.867075000
C	-4.174906000	-0.179609000	-5.182027000	C	3.253191000	2.665939000	5.158032000
C	-0.623389000	4.804316000	-2.526199000	C	4.223123000	1.726312000	4.886482000
C	0.685160000	4.106167000	-2.249463000	C	1.829564000	3.942411000	-3.063684000
C	-4.140286000	-2.927760000	-2.738427000	C	-1.697855000	-3.849159000	-3.219188000
C	-2.716987000	-3.302610000	-2.404993000	C	-1.990305000	-4.350981000	3.618662000
C	-3.536308000	-2.546172000	2.700052000	C	1.846030000	4.269032000	3.752431000
C	-3.506705000	-2.820169000	4.987655000	H	-0.875468000	4.445473000	-5.355500000
C	-4.452235000	-1.863015000	4.692796000	H	-3.036457000	2.851507000	-6.064440000
C	-5.311012000	-0.759348000	2.528509000	H	-5.187634000	2.287593000	-4.654494000
C	-4.596307000	0.537615000	2.250040000	H	-5.037604000	2.158607000	-2.870000000
C	-4.193365000	1.569408000	3.127781000	H	-3.989617000	-2.378211000	-5.546912000
C	-3.584373000	2.547131000	2.309746000	H	-4.167253000	0.330376000	-6.137301000
C	-3.019255000	3.900188000	2.645434000	H	-1.119187000	5.043188000	-1.574683000
C	-0.495711000	3.863776000	2.817728000	H	-0.441881000	5.741379000	-3.072480000
C	-0.291864000	3.966828000	5.112803000	H	-4.612803000	-3.709132000	-3.350581000
C	-1.634164000	3.899708000	4.813671000	H	-4.717902000	-2.804256000	-1.811585000
C	4.536940000	0.466370000	-2.727723000	H	-3.223268000	-3.253321000	5.938955000
C	4.371963000	1.610958000	-4.710731000	H	-6.225079000	-0.591841000	3.115967000
C	4.495920000	0.274846000	-5.021867000	H	-5.582570000	-1.242715000	1.579017000
C	4.744885000	-1.886531000	-3.679998000	H	-4.346665000	1.614113000	4.200570000
C	2.736528000	-3.173345000	-2.753153000	H	-2.818920000	4.451921000	1.715880000
C	1.825343000	-3.815382000	-4.763285000	H	-3.731324000	4.479964000	3.250736000
C	2.923192000	-3.034271000	-5.046300000	H	0.206573000	4.066165000	6.069266000
C	4.241941000	2.970591000	-2.528450000	H	-2.500253000	3.924435000	5.463354000
C	2.799843000	3.319816000	-2.244712000	H	4.307468000	2.478801000	-5.355117000
C	0.737731000	-4.720879000	-2.617921000	H	4.561244000	-0.215433000	-5.985267000
C	-0.587145000	-4.045327000	-2.365811000	H	5.421005000	-2.222907000	-4.477549000
C	0.377436000	-3.931015000	2.761353000	H	5.183647000	-2.111909000	-2.702361000
C	0.092850000	-3.981395000	5.047817000	H	1.149643000	-4.342177000	-5.425322000
C	1.443691000	-3.894875000	4.795117000	H	3.364457000	-2.767770000	-5.998747000
C	2.905597000	-3.922212000	2.678175000	H	4.783571000	2.838958000	-1.581067000
C	3.505539000	-2.572071000	2.388626000	H	4.724665000	3.774122000	-3.102683000
C	4.066174000	-1.604185000	3.251542000	H	0.585392000	-5.641874000	-3.199795000
C	4.554547000	-0.580595000	2.408464000	H	1.198904000	-4.989010000	-1.657077000
C	5.237596000	0.719932000	2.744404000	H	-0.437800000	-4.064250000	5.988252000

H	2.285746000	-3.887351000	5.475984000	H	-1.394604000	-1.080991000	-2.515304000
H	3.587897000	-4.522073000	3.298752000	H	-0.662534000	1.148126000	-0.492533000
H	2.736604000	-4.455046000	1.731660000	H	-1.677985000	-0.367155000	-0.152210000
H	4.135422000	-1.651230000	4.332946000	<u>2(E)-C₄H₈</u>			
H	5.545019000	1.227275000	1.818628000	Au	-0.905628000	3.612464000	0.761845000
H	6.125170000	0.557717000	3.372889000	Au	2.429546000	3.310596000	0.828949000
H	2.905017000	3.057478000	6.105877000	Au	4.745370000	0.904793000	-0.715869000
H	4.856350000	1.156551000	5.555248000	Au	-4.012057000	2.402855000	-0.856200000
H	1.951737000	4.265647000	-4.092286000	Au	-2.448984000	-3.293102000	0.808929000
H	-1.769990000	-4.107742000	-4.270455000	Au	0.858044000	-3.658197000	0.900602000
H	-2.115264000	-4.785829000	2.621198000	Au	3.913193000	-2.278367000	-0.642641000
H	-2.244756000	-5.102205000	4.378714000	Au	-4.651802000	-0.912705000	-0.853844000
H	2.008328000	4.706776000	2.761790000	N	-2.653654000	3.459237000	3.323432000
H	2.088337000	5.011701000	4.524862000	N	-0.547201000	3.916158000	3.755247000
H	-5.127231000	-1.318220000	5.341183000	N	1.966463000	3.615208000	3.808827000
H	-1.984302000	-0.508296000	4.359283000	N	3.856818000	2.557309000	3.459699000
C	-0.977609000	-0.199764000	4.035255000	N	-4.497054000	1.494232000	0.988900000
C	-0.881091000	-0.139683000	2.487630000	N	4.726999000	-0.017614000	1.184167000
C	0.478655000	0.333010000	2.011938000	N	4.670090000	0.373381000	-3.697572000
C	1.182733000	-0.266397000	1.027166000	N	3.912282000	2.394660000	-3.294005000
H	-0.768588000	0.791135000	4.476716000	N	1.522798000	3.551193000	-1.052521000
H	-0.243378000	-0.915174000	4.444151000	N	0.130556000	3.707247000	-1.071008000
H	-1.660502000	0.543083000	2.104060000	N	-2.503955000	3.451424000	-3.356777000
H	-1.085121000	-1.134646000	2.057579000	N	-3.982704000	1.909893000	-3.847894000
H	0.880423000	1.237845000	2.485650000	N	-3.985499000	-2.421287000	3.343629000
H	0.811046000	-1.149641000	0.506135000	N	-2.149608000	-3.523951000	3.813267000
H	2.134518000	0.123807000	0.683848000	N	0.349617000	-3.841200000	3.886300000
H	1.939046000	0.442658000	-3.990524000	N	2.454806000	-3.329537000	3.524068000
C	1.297223000	-0.094349000	-3.273755000	N	-4.780206000	0.118181000	0.983239000
C	-0.080806000	0.616792000	-3.132262000	N	4.353591000	-1.372165000	1.204246000
C	-0.958122000	-0.144001000	-2.158208000	N	4.231998000	-2.072680000	-3.651948000
C	-1.118956000	0.231196000	-0.869747000	N	2.712733000	-3.584918000	-3.183281000
H	1.160166000	-1.125970000	-3.637379000	N	-0.054193000	-3.779770000	-0.981306000
H	1.805619000	-0.138649000	-2.296088000	N	-1.441118000	-3.596681000	-1.025765000
H	-0.558722000	0.681752000	-4.127339000	N	-3.754841000	-2.505591000	-3.367883000
H	0.077416000	1.641231000	-2.764531000	N	-4.499778000	-0.503186000	-3.852733000

C	-1.439990000	3.667336000	2.704038000	C	1.827995000	-4.533178000	-2.440144000
C	-2.535229000	3.552143000	4.723353000	C	0.384574000	-4.101204000	-2.247872000
C	-1.218001000	3.842112000	4.995713000	C	-0.730930000	-4.111649000	-3.121493000
C	0.806968000	4.516241000	3.604393000	C	-1.856865000	-3.788906000	-2.318815000
C	2.815036000	3.160795000	2.794853000	C	-3.338355000	-3.735714000	-2.632470000
C	3.681429000	2.623418000	4.854339000	C	-4.320560000	-1.389765000	-2.787165000
C	2.498939000	3.293279000	5.076238000	C	-4.071610000	-1.086194000	-5.063947000
C	-3.959805000	3.313648000	2.605469000	C	-3.600612000	-2.340898000	-4.756718000
C	-4.322463000	1.883618000	2.295311000	C	-4.528807000	0.774954000	3.144724000
C	5.007697000	1.891026000	2.777963000	C	4.339731000	-0.610911000	3.344421000
C	4.705982000	0.443318000	2.477411000	C	5.242299000	-0.991043000	-3.545764000
C	4.462725000	1.293668000	-2.668593000	C	-5.044544000	0.874014000	-3.768873000
C	4.283498000	0.922932000	-4.937228000	H	-3.383783000	3.450061000	5.388578000
C	3.805354000	2.187142000	-4.683110000	H	-0.729124000	4.040301000	5.941561000
C	3.487453000	3.651109000	-2.598689000	H	0.883839000	5.322906000	4.346722000
C	1.996545000	3.737549000	-2.330778000	H	0.879717000	4.942975000	2.599030000
C	0.905585000	4.050811000	-3.179068000	H	4.411364000	2.234881000	5.553773000
C	-0.247062000	4.030360000	-2.353584000	H	2.030609000	3.592253000	6.005822000
C	-1.677190000	4.452850000	-2.623234000	H	-3.882798000	3.887413000	1.670860000
C	-3.494502000	2.678313000	-2.788380000	H	-4.722920000	3.787680000	3.240770000
C	-3.311979000	2.232610000	-5.045616000	H	5.882843000	1.993921000	3.436311000
C	-2.382644000	3.197223000	-4.734882000	H	5.204311000	2.433867000	1.842254000
C	-2.943499000	-3.093848000	2.746890000	H	4.403479000	0.398148000	-5.876491000
C	-3.859812000	-2.420437000	4.745416000	H	3.811501000	4.494866000	-3.225236000
C	-2.710696000	-3.117407000	5.042806000	H	4.035338000	3.690265000	-1.646288000
C	-0.996379000	-4.446116000	3.699055000	H	0.951353000	4.307044000	-4.232746000
C	1.278909000	-3.613040000	2.866835000	H	-2.187100000	4.650634000	-1.670005000
C	2.279391000	-3.362237000	4.920027000	H	-1.682574000	5.379150000	-3.217356000
C	0.961080000	-3.686573000	5.149496000	H	-3.571277000	1.796079000	-6.001430000
C	-5.096685000	-1.762643000	2.596127000	H	-1.692762000	3.738245000	-5.369803000
C	-4.802594000	-0.313635000	2.285187000	H	-4.601323000	-1.975791000	5.397565000
C	3.772405000	-3.159179000	2.838614000	H	-2.285919000	-3.385712000	6.002136000
C	4.120981000	-1.729245000	2.508778000	H	-1.112549000	-5.219595000	4.470926000
C	3.597093000	-2.710074000	-2.584764000	H	-1.028085000	-4.913366000	2.709575000
C	3.765681000	-2.582438000	-4.883430000	H	3.093413000	-3.199851000	5.615617000
C	2.810772000	-3.527301000	-4.587390000	H	0.436910000	-3.857410000	6.081704000

H	-5.244575000	-2.322885000	1.662186000	C	1.562524000	0.116922000	0.515939000
H	-6.005098000	-1.859218000	3.209266000	H	1.576748000	0.803456000	-3.570695000
H	4.533545000	-3.600685000	3.499617000	H	0.359548000	-0.472360000	-3.838780000
H	3.736307000	-3.749493000	1.911923000	H	1.150643000	-1.632762000	-1.655470000
H	4.165232000	-2.266700000	-5.839165000	H	1.849946000	1.323612000	-1.304103000
H	2.236528000	-4.172658000	-5.240204000	H	1.306617000	-0.912740000	0.791664000
H	1.855025000	-5.488817000	-2.985201000	H	0.797134000	0.794586000	0.923577000
H	2.290771000	-4.685829000	-1.454630000	H	2.504721000	0.380341000	1.003561000
H	-0.733089000	-4.364985000	-4.176896000	<u>2(Z)-C₄H₈</u>			
H	-3.915695000	-3.763450000	-1.697357000	Au	0.737082000	-4.043458000	-0.733611000
H	-3.629764000	-4.599260000	-3.248255000	Au	3.350197000	-2.301253000	-0.689235000
H	-4.180412000	-0.597040000	-6.023453000	Au	4.160529000	0.752822000	0.941221000
H	-3.221716000	-3.126133000	-5.398650000	Au	-2.405962000	-3.407486000	0.804699000
H	-4.499788000	0.764903000	4.228715000	Au	-3.497101000	2.422393000	-0.859040000
H	4.271534000	-0.575108000	4.426248000	Au	-0.706829000	3.982301000	-0.838176000
H	5.734416000	-1.060340000	-2.569826000	Au	2.400971000	3.406077000	0.866821000
H	5.979035000	-1.140071000	-4.346858000	Au	-4.064360000	-0.698585000	0.774707000
H	-5.590913000	0.990245000	-2.826983000	N	-0.786041000	-4.346688000	-3.374691000
H	-5.727107000	1.021938000	-4.616971000	N	1.380556000	-4.261737000	-3.700335000
H	3.441807000	2.949240000	-5.360752000	N	3.518023000	-2.978183000	-3.649233000
H	-1.342900000	-0.708980000	-2.488866000	N	4.518375000	-1.070484000	-3.244482000
C	-1.520022000	0.091317000	-1.755749000	N	-2.855176000	-2.665542000	-1.110667000
C	-1.259872000	-0.422909000	-0.352567000	N	3.777498000	1.509447000	-0.976350000
C	-1.633722000	0.151001000	0.812992000	N	4.166880000	1.268810000	3.942677000
C	-1.207592000	-0.333644000	2.184549000	N	4.311496000	-0.877112000	3.534533000
H	-0.848380000	0.930466000	-1.994825000	N	2.607300000	-2.822878000	1.204469000
H	-2.543736000	0.444010000	-1.890256000	N	1.436868000	-3.588909000	1.184280000
H	-0.620281000	-1.300926000	-0.292923000	N	-1.109285000	-4.339179000	3.423615000
H	-2.232375000	1.055293000	0.797616000	N	-3.002929000	-3.302940000	3.790162000
H	-0.605231000	-1.253088000	2.109196000	N	-4.371549000	1.004636000	-3.433119000
H	-2.082448000	-0.531571000	2.822752000	N	-3.289535000	2.859108000	-3.861908000
H	-0.599901000	0.439432000	2.692861000	N	-1.151480000	4.134905000	-3.844112000
H	2.074427000	-0.852416000	-4.005912000	N	0.988041000	4.273793000	-3.388606000
C	1.358024000	-0.264996000	-3.415156000	N	-3.630708000	-1.498806000	-1.113656000
C	1.394555000	-0.608249000	-1.940692000	N	3.006807000	2.676621000	-1.008581000
C	1.634711000	0.309676000	-0.976798000	N	2.817190000	3.351116000	3.883794000

N	0.937020000	4.359479000	3.393391000	C	2.269727000	4.419607000	-2.633976000
N	-1.565048000	3.638385000	1.043881000	C	2.950504000	3.114414000	-2.309618000
N	-2.764358000	2.917259000	1.037607000	C	2.030644000	3.763134000	2.809292000
N	-4.482443000	0.940111000	3.342617000	C	2.207430000	3.697693000	5.107672000
N	-4.340632000	-1.205339000	3.760372000	C	1.023552000	4.328713000	4.796836000
C	0.410021000	-4.271835000	-2.700332000	C	-0.172950000	4.985222000	2.618807000
C	-0.584246000	-4.374424000	-4.766203000	C	-1.323374000	4.053451000	2.330748000
C	0.776517000	-4.323421000	-4.973345000	C	-2.361222000	3.583769000	3.168403000
C	2.844768000	-4.285815000	-3.469048000	C	-3.246285000	2.876536000	2.321924000
C	3.848824000	-2.097450000	-2.621213000	C	-4.581109000	2.236030000	2.607429000
C	4.605006000	-1.286710000	-4.632396000	C	-4.343855000	-0.278278000	2.719354000
C	3.976740000	-2.485228000	-4.889042000	C	-4.474021000	-0.553967000	5.004994000
C	-2.112375000	-4.451974000	-2.693382000	C	-4.560402000	0.794686000	4.740379000
C	-2.783130000	-3.132356000	-2.401629000	C	-3.518247000	-2.267674000	-3.244669000
C	5.130352000	0.078990000	-2.510198000	C	3.689374000	2.227836000	-3.126388000
C	4.190790000	1.231952000	-2.256547000	C	4.160927000	2.738516000	3.773173000
C	4.259105000	0.344464000	2.904442000	C	-4.329400000	-2.676870000	3.590944000
C	4.169272000	0.614406000	5.192260000	H	-1.398091000	-4.464060000	-5.474868000
C	4.256584000	-0.735399000	4.932793000	H	1.344937000	-4.366148000	-5.894073000
C	4.415850000	-2.175194000	2.806231000	H	3.289015000	-4.993083000	-4.182274000
C	3.082450000	-2.806476000	2.493481000	H	3.024472000	-4.627016000	-2.443942000
C	2.207706000	-3.553960000	3.316198000	H	5.125697000	-0.610709000	-5.299330000
C	1.190276000	-4.032988000	2.459031000	H	3.862194000	-3.029651000	-5.818271000
C	0.043524000	-4.976312000	2.722126000	H	-1.947412000	-4.989110000	-1.748423000
C	-2.169081000	-3.756146000	2.769600000	H	-2.756276000	-5.068407000	-3.337296000
C	-2.453466000	-3.609356000	5.052638000	H	5.996513000	0.412770000	-3.099723000
C	-1.260886000	-4.257617000	4.819563000	H	5.490379000	-0.309100000	-1.546425000
C	-3.803436000	2.095726000	-2.816771000	H	4.151297000	1.145436000	6.135916000
C	-4.224783000	1.072319000	-4.830320000	H	5.020279000	-2.851291000	3.428142000
C	-3.548546000	2.240680000	-5.103026000	H	4.957562000	-1.982189000	1.869342000
C	-2.628188000	4.172720000	-3.707997000	H	2.321806000	-3.757911000	4.375777000
C	-0.244403000	4.166807000	-2.785205000	H	-0.333554000	-5.366120000	1.765907000
C	0.870289000	4.303273000	-4.790161000	H	0.376061000	-5.822076000	3.341140000
C	-0.473627000	4.219273000	-5.078493000	H	-2.959136000	-3.388796000	5.984499000
C	-4.998390000	-0.128357000	-2.693391000	H	-0.550375000	-4.691293000	5.512130000
C	-4.041283000	-1.259641000	-2.401820000	H	-4.637919000	0.327396000	-5.498856000

H	-3.280227000	2.687810000	-6.052100000	H	-0.015290000	-0.461339000	4.405181000
H	-3.017769000	4.845225000	-4.484329000	C	0.776306000	-0.840246000	-3.421367000
H	-2.874845000	4.567254000	-2.716668000	C	-0.107523000	-0.737772000	-2.399462000
H	1.723206000	4.416928000	-5.447630000	H	1.386212000	-1.739651000	-3.481305000
H	-0.986980000	4.255961000	-6.031324000	H	-0.178618000	-1.556069000	-1.679832000
H	-5.387556000	0.273721000	-1.747396000	C	0.989335000	0.193692000	-4.512301000
H	-5.843163000	-0.488806000	-3.298124000	H	2.048173000	0.502532000	-4.554667000
H	2.929681000	5.056116000	-3.241293000	H	0.733137000	-0.221586000	-5.504932000
H	2.037407000	4.949124000	-1.698916000	H	0.376074000	1.093986000	-4.348587000
H	2.669287000	3.511205000	6.069329000	C	-1.033774000	0.442408000	-2.182198000
H	0.277738000	4.779657000	5.439566000	H	-0.476379000	1.391119000	-2.122015000
H	-0.522334000	5.854197000	3.195426000	H	-1.751057000	0.534056000	-3.012629000
H	0.252322000	5.343553000	1.670424000	H	-1.605662000	0.328098000	-1.253224000
H	-2.480422000	3.769945000	4.230606000	<u>2Iso-butylene@PPX</u>			
H	-5.098368000	2.033721000	1.658598000	Au	0.341057000	-3.989658000	-0.749838000
H	-5.208351000	2.906180000	3.212940000	Au	3.241856000	-2.631381000	-0.755662000
H	-4.540169000	-1.087219000	5.945230000	Au	4.384027000	0.379061000	0.823158000
H	-4.708539000	1.633129000	5.409635000	Au	-2.755287000	-3.072855000	0.823280000
H	-3.680412000	-2.379198000	-4.311549000	Au	-3.414456000	2.705146000	-0.862319000
H	3.868438000	2.316443000	-4.192487000	Au	-0.319833000	3.839412000	-0.885797000
H	4.569116000	2.974993000	2.784860000	Au	2.838146000	3.152086000	0.745804000
H	4.797703000	3.175275000	4.554349000	Au	-4.363147000	-0.288526000	0.784063000
H	-4.671318000	-2.912175000	2.577544000	N	-1.313350000	-4.178856000	-3.335692000
H	-5.021788000	-3.106245000	4.327713000	N	0.845529000	-4.251454000	-3.727429000
H	4.321515000	-1.577769000	5.610137000	N	3.125561000	-3.200990000	-3.733646000
C	-0.458887000	-0.407320000	1.124718000	N	4.407483000	-1.460809000	-3.354238000
C	-0.882013000	-0.480840000	2.412125000	N	-3.289476000	-2.361034000	-1.075074000
H	-1.005302000	-0.982794000	0.371781000	N	4.185998000	1.230755000	-1.082822000
H	-1.743374000	-1.119132000	2.623177000	N	4.423860000	0.887393000	3.819581000
C	0.708179000	0.405756000	0.615928000	N	4.358599000	-1.265880000	3.425879000
H	1.342184000	0.756699000	1.442112000	N	2.474702000	-3.113463000	1.132278000
H	1.336269000	-0.184202000	-0.071195000	N	1.211614000	-3.709462000	1.134611000
H	0.365392000	1.295064000	0.057493000	N	-1.434020000	-4.040099000	3.425394000
C	-0.304505000	0.252017000	3.610864000	N	-3.260399000	-2.891803000	3.816118000
H	0.578156000	0.856442000	3.348749000	N	-4.423182000	1.338820000	-3.428990000
H	-1.061090000	0.932963000	4.044087000	N	-3.059123000	2.998667000	-3.864480000

N	-0.761413000	4.005392000	-3.880630000	C	0.163760000	3.982399000	-2.832977000
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N	-4.017837000	-1.166290000	-1.088047000	C	-0.094526000	4.043503000	-5.124302000
N	3.522949000	2.460153000	-1.107958000	C	-5.228703000	0.313658000	-2.696721000
N	3.210725000	3.054912000	3.755428000	C	-4.424115000	-0.924769000	-2.376211000
N	1.379806000	4.155203000	3.268903000	C	2.701607000	4.155114000	-2.733906000
N	-1.255091000	3.644720000	0.988959000	C	3.385526000	2.847550000	-2.418075000
N	-2.548273000	3.105965000	1.009747000	C	2.447049000	3.513331000	2.683391000
N	-4.474023000	1.417425000	3.346268000	C	2.610681000	3.412024000	4.979580000
N	-4.497409000	-0.728829000	3.784752000	C	1.459767000	4.102575000	4.672651000
C	-0.093736000	-4.190338000	-2.696896000	C	0.313261000	4.863000000	2.503768000
C	-1.154545000	-4.212658000	-4.734239000	C	-0.946801000	4.063928000	2.262102000
C	0.199503000	-4.260312000	-4.981122000	C	-2.036731000	3.774406000	3.117827000
C	2.307932000	-4.426261000	-3.546018000	C	-3.021315000	3.174093000	2.297458000
C	3.661740000	-2.420101000	-2.707571000	C	-4.427239000	2.714457000	2.607404000
C	4.344400000	-1.622200000	-4.750841000	C	-4.497341000	0.185788000	2.733439000
C	3.541349000	-2.715376000	-4.990351000	C	-4.480246000	-0.057910000	5.024843000
C	-2.626474000	-4.206517000	-2.621356000	C	-4.461524000	1.290502000	4.747590000
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C	5.214221000	-0.416482000	-2.649758000	C	3.972936000	1.865725000	-3.250462000
C	4.456851000	0.862012000	-2.377666000	C	4.513285000	2.355015000	3.648760000
C	4.419829000	-0.049796000	2.787803000	C	-4.562225000	-2.202222000	3.643272000
C	4.366993000	0.244365000	5.072540000	H	-1.993077000	-4.245839000	-5.418694000
C	4.323967000	-1.109279000	4.823070000	H	0.733791000	-4.344624000	-5.919327000
C	4.329073000	-2.577213000	2.713739000	H	2.648350000	-5.166184000	-4.283354000
C	2.934430000	-3.076015000	2.425338000	H	2.484483000	-4.805481000	-2.533978000
C	1.959642000	-3.648462000	3.275060000	H	4.892946000	-0.990469000	-5.438373000
C	0.893255000	-4.034444000	2.428885000	H	3.276437000	-3.195183000	-5.924321000
C	-0.367613000	-4.811195000	2.717320000	H	-2.454485000	-4.716361000	-1.662609000
C	-2.471031000	-3.401490000	2.785892000	H	-3.307578000	-4.822910000	-3.226455000
C	-2.703769000	-3.216051000	5.070495000	H	6.099768000	-0.219461000	-3.271719000
C	-1.555655000	-3.935232000	4.822954000	H	5.545932000	-0.851241000	-1.695927000
C	-3.734016000	2.363298000	-2.820656000	H	4.406981000	0.780771000	6.012428000
C	-4.200606000	1.327471000	-4.818503000	H	4.875970000	-3.299030000	3.337764000
C	-3.348752000	2.372531000	-5.094842000	H	4.874341000	-2.446968000	1.768037000
C	-2.227614000	4.216296000	-3.731808000	H	2.035210000	-3.804955000	4.346120000

H	-0.800575000	-5.162630000	1.770052000	H	0.724388000	1.543441000	3.526450000
H	-0.139042000	-5.687543000	3.341846000	H	1.462980000	0.018779000	4.059480000
H	-3.177613000	-2.958769000	6.009606000	H	1.992696000	0.780548000	2.524322000
H	-0.860258000	-4.404337000	5.507717000	H	-1.294721000	-0.624784000	4.046514000
H	-4.686026000	0.622749000	-5.482004000	H	-1.702462000	0.842429000	3.125572000
H	-2.970969000	2.733328000	-6.043169000	H	-2.018248000	-0.765718000	2.415079000
H	-2.534048000	4.923041000	-4.515381000	C	0.394167000	-1.191660000	-3.007318000
H	-2.415668000	4.656062000	-2.746757000	C	0.078637000	-0.156062000	-2.195229000
H	2.103539000	4.107157000	-5.525939000	H	-0.362974000	-1.678634000	-3.623291000
H	-0.616367000	4.108983000	-6.071002000	H	1.419542000	-1.536398000	-3.091449000
H	-5.584417000	0.778047000	-1.766010000	C	1.115779000	0.630869000	-1.429433000
H	-6.096688000	0.065697000	-3.324349000	C	-1.323637000	0.379110000	-2.081288000
H	3.343106000	4.788730000	-3.364037000	H	1.368259000	1.523687000	-2.016927000
H	2.495078000	4.690390000	-1.796045000	H	0.732740000	0.991288000	-0.462579000
H	3.058513000	3.192564000	5.940801000	H	2.029806000	0.050459000	-1.252537000
H	0.736428000	4.583853000	5.318837000	H	-1.692631000	0.310550000	-1.042958000
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H	0.750733000	5.152158000	1.537777000	H	-2.024691000	-0.142777000	-2.743381000
H	-2.120689000	4.010284000	4.173705000				
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H	-4.142160000	-2.094710000	-4.270073000				
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H	4.314309000	-1.949665000	5.505905000				
C	0.333491000	-0.813867000	1.239601000				
C	0.060356000	-0.185082000	2.406106000				
H	-0.427118000	-1.359058000	0.677615000				
H	1.337666000	-0.798107000	0.817225000				
C	1.127471000	0.581244000	3.168314000				
C	-1.320524000	-0.188932000	3.030264000				