

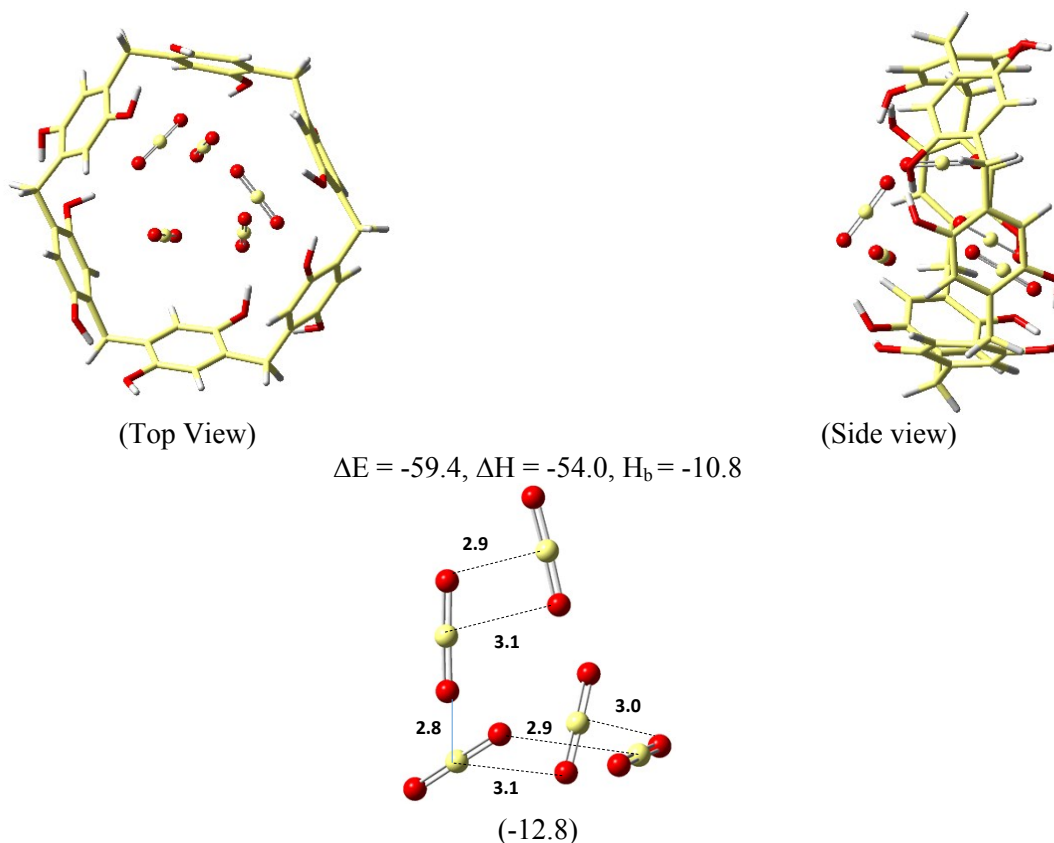
## Electronic Supplementary Information

### The role of non-covalent interaction for the adsorption of CO<sub>2</sub> and hydrocarbons with per-hydroxylated pillar[6]arene: A Computational Study

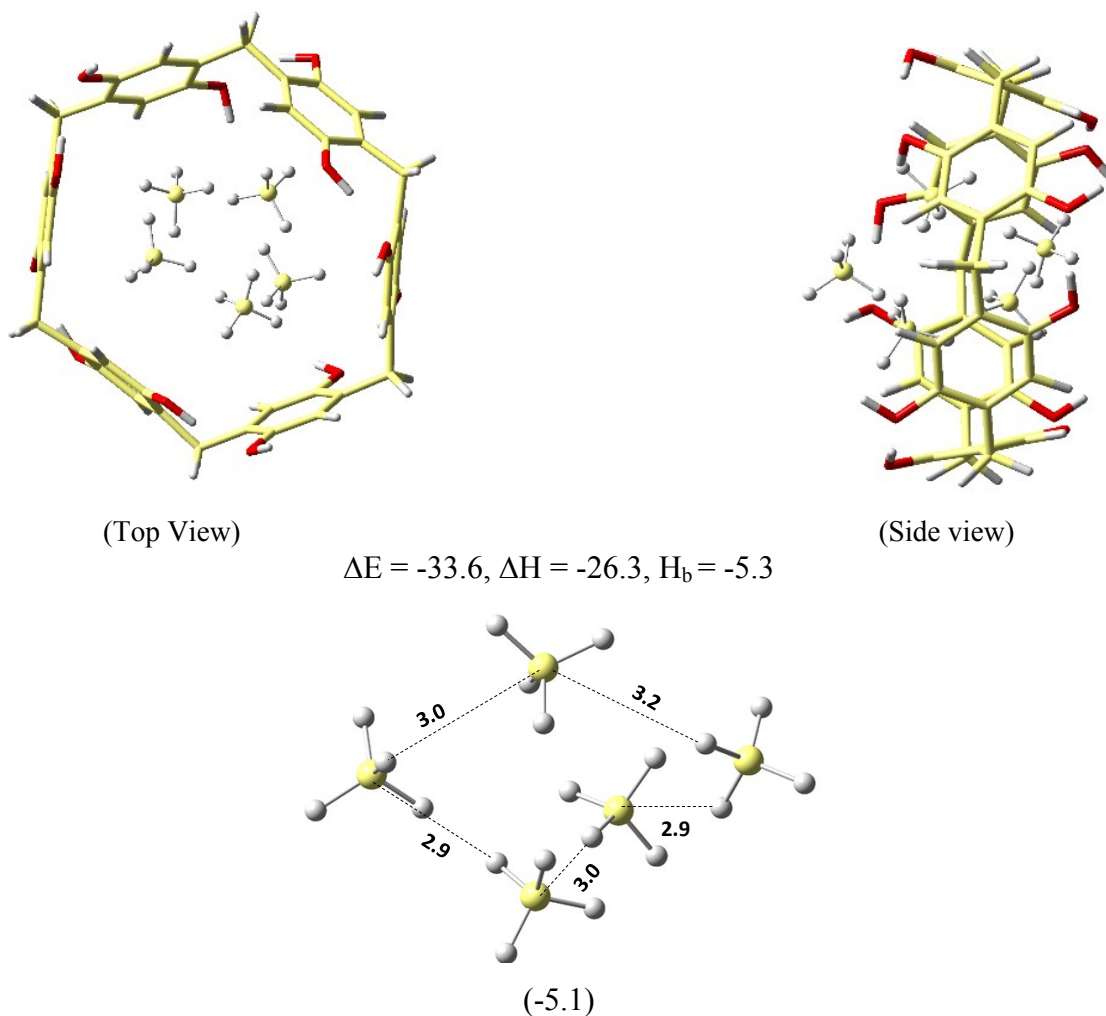
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**Figure S1:** B3LYP-D3/6-31G(d) calculated optimized structures of PA[6] with five CO<sub>2</sub> gas molecules and cooperative intermolecular interactions among the CO<sub>2</sub> gas molecules inside PA[6] cavity. Binding electronic energies ( $\Delta E$ ), binding enthalpies ( $\Delta H$ ), and binding enthalpies per gas molecule ( $H_b$ ) are given in kcal/mol. All the distances are in angstroms (Å) unit and aromatic rings of PA[6] are marked numerically.



**Figure S2:** B3LYP-D3/6-31G(d) calculated optimized structures of PA[6] with five CH<sub>4</sub> gas molecules and cooperative intermolecular interactions among the CH<sub>4</sub> gas molecules inside PA[6] cavity. Binding electronic energies ( $\Delta E$ ), binding enthalpies ( $\Delta H$ ), and binding enthalpies per gas molecule ( $H_b$ ) are given in kcal/mol. All the distances are in angstroms ( $\text{\AA}$ ) unit and aromatic rings of PA[6] are marked numerically.

**Table S1:** Molecular graphs (network of bond paths linking pairs of neighboring nuclei) of four CO<sub>2</sub> adsorbed inside PA[6] (top view for the better clarity). Small red dots indicates bond critical points (3, -1).

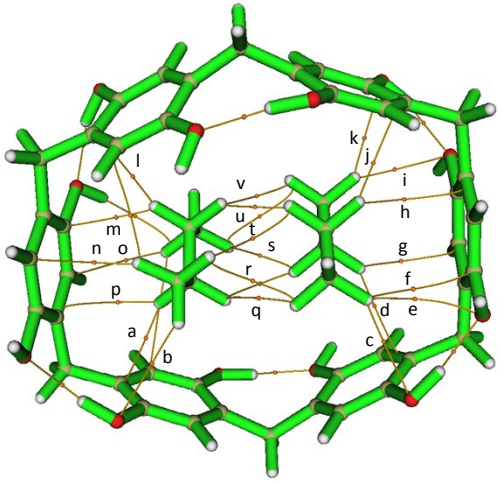
4 CO <sub>2</sub> inside P[6]		$\rho(r_c)$	$\nabla^2\rho(r_c)$	$ V(r_c)/G(r_c) $
	a	0.00753	0.02577	0.83
	b	0.00695	0.02455	0.69
	c	0.01626	0.06031	0.95
	d	0.00579	0.01923	0.81
	e	0.05681	0.01899	0.80
	f	0.00626	0.02223	0.77

	g	0.01660	0.06149	0.95
	h	0.00678	0.02395	0.68
	i	0.00735	0.02550	0.83
	j	0.00647	0.02252	0.79
	k	0.00597	0.01954	0.82
	l	0.00522	0.01754	0.79
	m	0.00726	0.02532	0.82
	n	0.01018	0.04292	0.82
	o	0.00966	0.03915	0.84
	p	0.00950	0.03842	0.84
	q	0.01022	0.04336	0.82

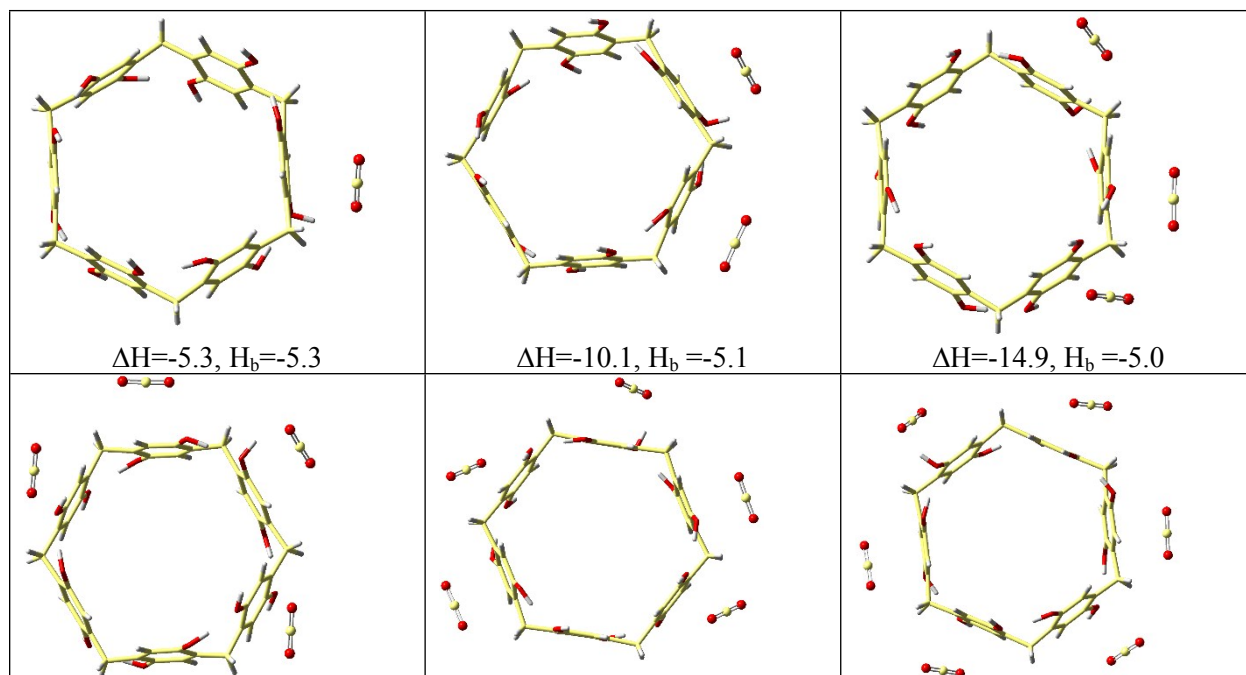
**Table S2:** Molecular graphs (network of bond paths linking pairs of neighboring nuclei) of four CH<sub>4</sub> adsorbed inside PA[6] (top view for the better clarity). Small red dots indicates critical points.

4 CH <sub>4</sub> inside P[6]		$\rho(r_c)$	$\nabla^2\rho(r_c)$	$ V(r_c)/G(r_c) $
	a	0.00777	0.02726	0.85
	b	0.00807	0.02773	0.86
	c	0.00533	0.01793	0.72
	d	0.00854	0.02834	0.88
	e	0.00305	0.00964	0.73
	f	0.00506	0.01661	0.72
	g	0.00518	0.01605	0.72
	h	0.00465	0.01502	0.72
	i	0.00608	0.01914	0.73
	j	0.00659	0.02769	0.68
	k	0.00296	0.00954	0.67
	l	0.00512	0.01697	0.73
	m	0.00435	0.01427	0.74
	n	0.00324	0.01172	0.57
	o	0.00509	0.01806	0.67
	p	0.00240	0.00810	0.71
	q	0.00424	0.01511	0.64
	r	0.00421	0.01527	0.64

**Table S3:** Molecular graphs (network of bond paths linking pairs of neighboring nuclei) of two n-butane adsorbed inside PA[6] (top view for the better clarity). Small red dots indicates critical points

2 n-butane inside P[6]		$\rho(r_c)$	$\nabla^2\rho(r_c)$	$ V(r_c)/G(r_c) $
	a	0.00924	0.02959	0.78
	b	0.00268	0.01133	0.67
	c	0.00596	0.02204	0.79
	d	0.00749	0.02306	0.75
	e	0.00518	0.02028	0.74
	f	0.00518	0.01961	0.70
	g	0.00754	0.02340	0.76
	h	0.00634	0.02014	0.74
	i	0.00679	0.02504	0.82
	j	0.00864	0.02723	0.77
	k	0.00685	0.02490	0.82
	l	0.00847	0.02649	0.77
	m	0.00811	0.02846	0.74
	n	0.00592	0.01753	0.76
	o	0.00600	0.01964	0.71
	p	0.00667	0.02149	0.74
	q	0.00436	0.01605	0.67
	r	0.00528	0.01958	0.67
	s	0.00498	0.01863	0.68
t	0.00361	0.01311	0.69	
u	0.00909	0.03249	0.76	
v	0.00551	0.02076	0.68	

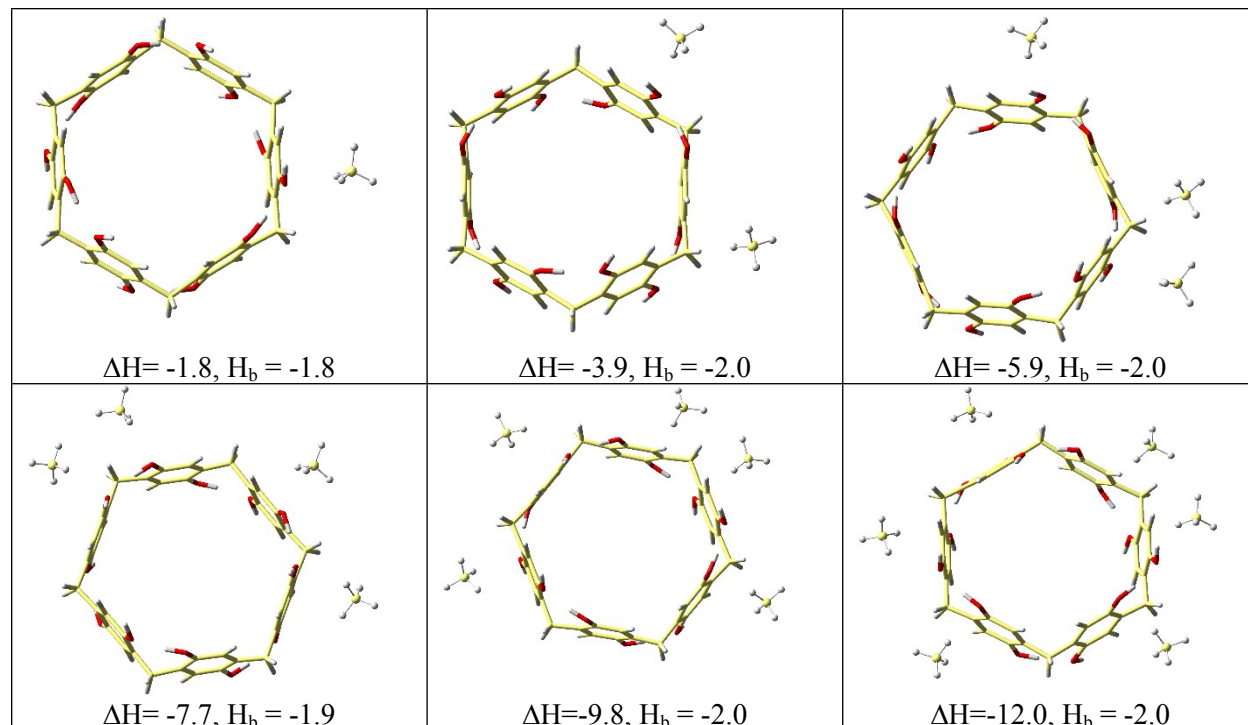
*Outside the PA[6] cavity*



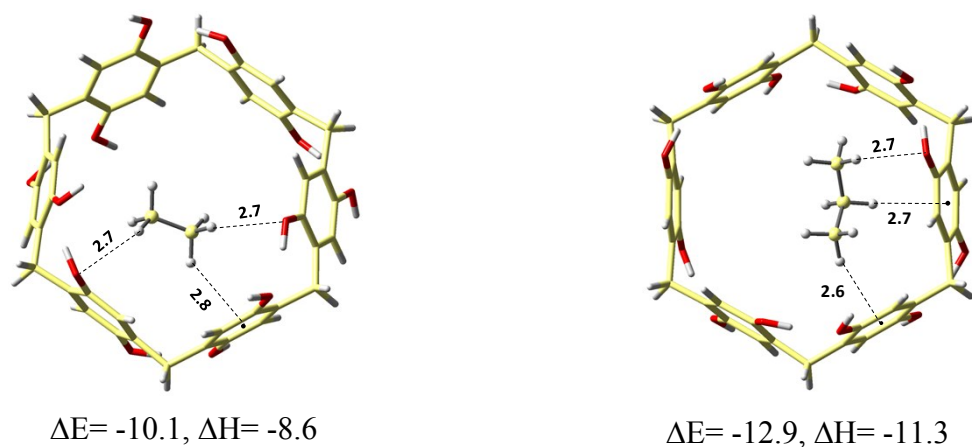
$\Delta H = -19.6$ , $H_b = -4.9$	$\Delta H = -24.4$ , $H_b = -4.9$	$\Delta H = -29.3$ , $H_b = -4.9$
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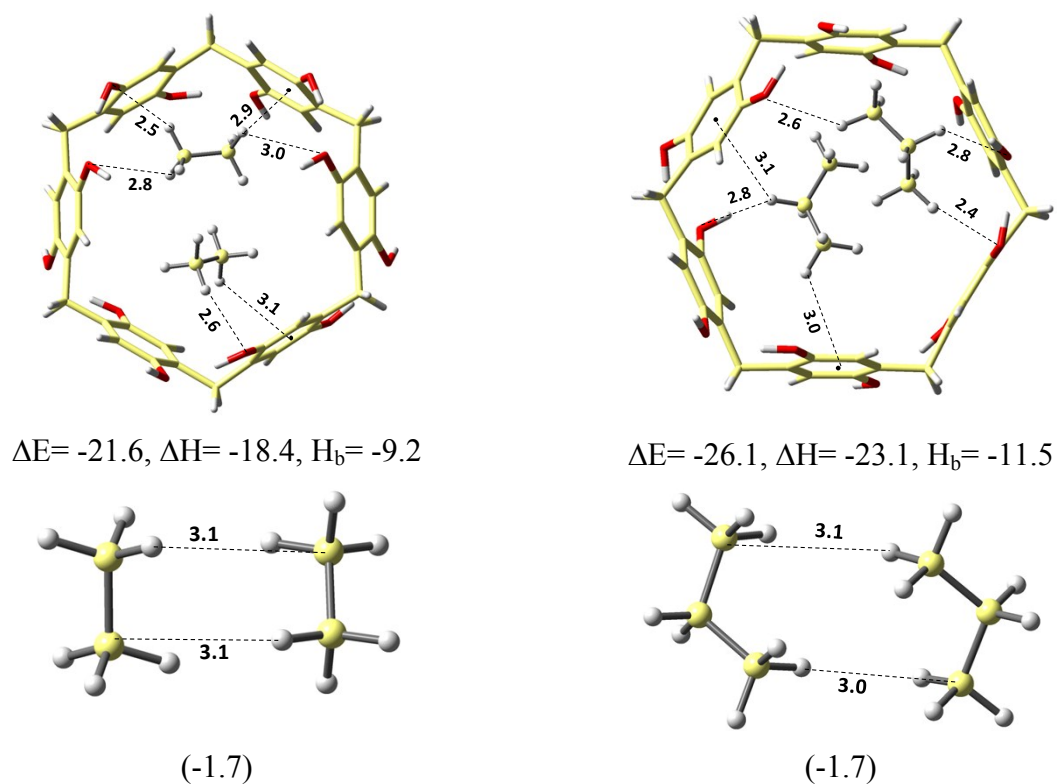
**Figure S3:** B3LYP-D3/6-31G(d) calculated optimized structures of PA[6] with CO<sub>2</sub> interacting with the outside the cavity of PA[6]. Binding enthalpies ( $\Delta H$ ) and binding enthalpies per gas molecule ( $H_b$ ) are given in kcal/mol.

*Outside the PA[6] cavity*



**Figure S4:** B3LYP-D3/6-31G(d) calculated optimized structures of PA[6] with CH<sub>4</sub> interacting with the outside the cavity of PA[6]. Binding enthalpies ( $\Delta H$ ) and binding enthalpies per gas molecule ( $H_b$ ) are given in kcal/mol.





**Figure S5:** B3LYP-D3/6-31G(d) calculated optimized structures of PA[6] with  $C_2H_6$  and  $C_3H_8$  (top view for the better clarity). Binding electronic energies ( $\Delta E$ ), binding enthalpies ( $\Delta H$ ) are given in kcal/mol. All the distances are in angstroms ( $\text{\AA}$ ) unit.

**Table S4:** B3LYP-D3/6-31G(d) calculated binding free energies ( $\Delta G$ , kcal/mol) for the adsorption of the  $CO_2$ ,  $CH_4$ , ethane, propane and butane with PA[6]

PA[6] host:	No. of guest molecules				
	1 ( $\Delta G$ )	2 ( $\Delta G$ )	3 ( $\Delta G$ )	4 ( $\Delta G$ )	5 ( $\Delta G$ )
$CO_2$	0.4	-1.7	-1.9	-2.3	-5.1
$CH_4$	3.1	4.6	7.2	8.7	14.5
$C_2H_6$	1.7	2.4	-	-	-
$C_3H_8$	0.2	-0.2	-	-	-
n- $C_4H_{10}$	-24.6	-44.5	-	-	-

**Table S5:** Cartesian coordinates of optimized structures of CO<sub>2</sub>, CH<sub>4</sub> and n-butane adsorbed inside the PA[6] host

*Inside the PA[6] cavity*

PA[6]+1CO <sub>2</sub>				PA[6]+2CO <sub>2</sub>			
O	-6.187256000000	0.262835000000	-1.919778000000	O	1.710638000000	-3.924985000000	-2.481451000000
O	-3.977610000000	-2.004128000000	2.625867000000	O	3.584860000000	-3.652388000000	2.726284000000
O	-0.665534000000	-4.657131000000	-2.653660000000	O	5.678212000000	1.817401000000	-1.893894000000
O	-2.817702000000	-4.575537000000	2.449030000000	O	4.295729000000	-0.860464000000	2.754316000000
O	2.003324000000	-3.706039000000	-2.662916000000	O	3.001960000000	2.710314000000	-2.088707000000
O	4.327172000000	-3.474995000000	2.366773000000	O	1.014916000000	6.117991000000	1.810406000000
C	-5.625113000000	-0.355164000000	-0.807567000000	C	2.235988000000	-3.894299000000	-1.194302000000
C	-5.370298000000	0.446775000000	0.311365000000	C	1.596843000000	-4.641126000000	-0.195380000000
C	-4.803553000000	-0.165317000000	1.427728000000	C	2.083923000000	-4.522032000000	1.107901000000
H	-4.580322000000	0.423946000000	2.312309000000	H	1.589113000000	-5.042959000000	1.922516000000
C	-4.506984000000	-1.532269000000	1.461587000000	C	3.199775000000	-3.736682000000	1.414085000000
C	-4.794350000000	-2.334853000000	0.341288000000	C	3.917615000000	-3.116720000000	0.378660000000
C	-5.347071000000	-1.717521000000	-0.787164000000	C	3.397634000000	-3.181842000000	-0.917300000000
H	-5.585617000000	-2.325826000000	-1.659277000000	H	3.916695000000	-2.675967000000	-1.727606000000
C	-4.544301000000	-3.833053000000	0.335881000000	C	5.249931000000	-2.428197000000	0.624866000000
H	-4.902423000000	-4.276619000000	1.271407000000	H	5.647617000000	-2.736127000000	1.596668000000
H	-5.148391000000	-4.281452000000	-0.460668000000	H	5.966274000000	-2.778372000000	-0.127129000000
C	-3.094146000000	-4.230954000000	0.114956000000	C	5.163366000000	-0.921288000000	0.545935000000
C	-2.266341000000	-4.610309000000	1.177208000000	C	4.657727000000	-0.166922000000	1.612219000000
C	-0.955990000000	-5.029191000000	0.957207000000	C	4.542624000000	1.217163000000	1.518837000000
H	-0.341854000000	-5.344375000000	1.798963000000	H	4.146100000000	1.788285000000	2.356457000000
C	-0.408388000000	-5.063827000000	-0.326602000000	C	4.899069000000	1.899180000000	0.351537000000
C	-1.220940000000	-4.636189000000	-1.384025000000	C	5.377236000000	1.140599000000	-0.721001000000
C	-2.538292000000	-4.239413000000	-1.166935000000	C	5.521796000000	-0.241402000000	-0.617862000000
H	-3.156269000000	-3.933809000000	-2.009838000000	H	5.902879000000	-0.808025000000	-1.465518000000
C	1.007997000000	-5.561027000000	-0.556895000000	C	4.751431000000	3.405449000000	0.245597000000
H	1.194369000000	-6.387451000000	0.137455000000	H	5.137373000000	3.858591000000	1.165048000000
H	1.084124000000	-5.985594000000	-1.563694000000	H	5.395662000000	3.771115000000	-0.562440000000
C	2.099367000000	-4.521622000000	-0.355678000000	C	3.326622000000	3.895464000000	0.039631000000
C	2.715105000000	-4.394203000000	0.891910000000	C	2.744918000000	4.737028000000	0.990156000000
H	2.378801000000	-4.997651000000	1.731035000000	H	3.294720000000	5.008206000000	1.887434000000

C	3.785028000000	-3.525207000000	1.106947000000	C	1.465742000000	5.274268000000	0.829888000000
C	4.300104000000	-2.784220000000	0.028784000000	C	0.735265000000	4.989455000000	-0.337543000000
C	3.642982000000	-2.856947000000	-1.202566000000	C	1.297728000000	4.111585000000	-1.268195000000
H	3.999127000000	-2.271007000000	-2.045710000000	H	0.758163000000	3.866321000000	-2.179060000000
C	2.543458000000	-3.695756000000	-1.406858000000	C	2.568470000000	3.563459000000	-1.099316000000
C	5.553169000000	-1.935895000000	0.174174000000	C	-0.589158000000	5.675443000000	-0.641135000000
H	6.103626000000	-2.248347000000	1.067657000000	H	-0.629682000000	6.626269000000	-0.097789000000
H	6.211241000000	-2.131726000000	-0.679212000000	H	-0.606217000000	5.927837000000	-1.706827000000
H	-2.125879000000	-4.741401000000	3.108142000000	H	3.834737000000	-0.264767000000	3.364298000000
H	1.110271000000	-4.099501000000	-2.658454000000	H	3.973002000000	2.620628000000	-2.087604000000
H	-3.687542000000	-2.933050000000	2.551940000000	H	3.943129000000	-2.756963000000	2.877678000000
H	-6.214590000000	-0.365150000000	-2.657509000000	H	1.957619000000	-3.101383000000	-2.933129000000
H	-1.275134000000	-4.245233000000	-3.284926000000	H	5.871563000000	1.173434000000	-2.593148000000
H	4.598714000000	-2.549824000000	2.530534000000	H	0.043944000000	6.031882000000	1.876425000000
O	4.298414000000	-0.686401000000	2.425132000000	O	-1.698098000000	5.505489000000	1.963709000000
O	5.478785000000	2.457427000000	-1.989043000000	O	-4.246347000000	2.826002000000	-2.159087000000
O	0.206197000000	6.178660000000	1.773029000000	O	-3.730158000000	-1.713845000000	2.314994000000
O	2.801855000000	3.124960000000	-2.059638000000	O	-6.450673000000	1.098620000000	-1.614837000000
O	-2.341478000000	4.980159000000	2.087599000000	O	-3.384732000000	-4.467429000000	2.379746000000
O	-4.478291000000	2.461966000000	-2.367589000000	O	-1.085966000000	-4.176024000000	-2.657964000000
C	4.617014000000	0.121870000000	1.331527000000	C	-2.348585000000	4.787033000000	0.968392000000
C	5.263485000000	-0.450542000000	0.227227000000	C	-1.831148000000	4.861205000000	-0.330881000000
C	5.548869000000	0.377265000000	-0.858600000000	C	-2.512689000000	4.173674000000	-1.333951000000
H	6.018072000000	-0.028803000000	-1.749788000000	H	-2.155603000000	4.215517000000	-2.358863000000
C	5.200637000000	1.730234000000	-0.863264000000	C	-3.672742000000	3.432458000000	-1.080082000000
C	4.594237000000	2.307994000000	0.267533000000	C	-4.180395000000	3.361970000000	0.229583000000
C	4.304185000000	1.478260000000	1.355591000000	C	-3.495722000000	4.050034000000	1.238691000000
H	3.833351000000	1.893054000000	2.244038000000	H	-3.886175000000	4.019024000000	2.255403000000
C	4.303236000000	3.794899000000	0.328431000000	C	-5.436611000000	2.578365000000	0.564099000000
H	4.928049000000	4.303692000000	-0.415207000000	H	-6.269207000000	2.905520000000	-0.069060000000
H	4.623879000000	4.174533000000	1.305272000000	H	-5.730152000000	2.814969000000	1.592771000000
C	2.854264000000	4.191391000000	0.113698000000	C	-5.274029000000	1.072146000000	0.445578000000
C	2.159847000000	3.853689000000	-1.056282000000	C	-5.809416000000	0.360091000000	-0.632578000000
C	0.859787000000	4.301396000000	-1.274633000000	C	-5.702173000000	-1.028066000000	-0.712319000000
H	0.370032000000	4.036150000000	-2.207285000000	H	-6.156387000000	-1.554894000000	-1.550045000000



C	0.188708000000	5.093357000000	-0.339455000000	C	-5.022737000000	-1.757030000000	0.266635000000
C	0.872554000000	5.399187000000	0.843304000000	C	-4.431182000000	-1.038079000000	1.315703000000
C	2.177818000000	4.960821000000	1.064322000000	C	-4.570926000000	0.342747000000	1.407556000000
H	2.688240000000	5.240916000000	1.984695000000	H	-4.117563000000	0.855620000000	2.251161000000
C	-1.214042000000	5.612790000000	-0.609541000000	C	-4.938102000000	-3.269210000000	0.196084000000
H	-1.268905000000	5.911203000000	-1.661853000000	H	-5.547875000000	-3.612713000000	-0.647046000000
H	-1.380090000000	6.525472000000	-0.026102000000	H	-5.388193000000	-3.700358000000	1.097406000000
C	-2.327820000000	4.613822000000	-0.340411000000	C	-3.530311000000	-3.811358000000	0.036679000000
C	-2.916442000000	3.929291000000	-1.407271000000	C	-2.889813000000	-3.745926000000	-1.202694000000
H	-2.563978000000	4.098265000000	-2.421413000000	H	-3.385222000000	-3.282178000000	-2.051604000000
C	-3.981193000000	3.042905000000	-1.233157000000	C	-1.611468000000	-4.274370000000	-1.402206000000
C	-4.497828000000	2.834302000000	0.059883000000	C	-0.946643000000	-4.904830000000	-0.330868000000
C	-3.891804000000	3.498284000000	1.128868000000	C	-1.574848000000	-4.933846000000	0.916270000000
H	-4.269083000000	3.358338000000	2.138260000000	H	-1.078561000000	-5.392625000000	1.767015000000
C	-2.817700000000	4.373851000000	0.956482000000	C	-2.842106000000	-4.387835000000	1.119300000000
C	-5.694270000000	1.931830000000	0.314655000000	C	0.417262000000	-5.547195000000	-0.508885000000
H	-6.481496000000	2.134743000000	-0.420300000000	H	0.511866000000	-5.929709000000	-1.530629000000
H	-6.115604000000	2.189329000000	1.291983000000	H	0.476193000000	-6.417726000000	0.153079000000
H	2.578163000000	2.183009000000	-1.952814000000	H	-6.689884000000	0.515854000000	-2.352312000000
H	-1.521636000000	5.476962000000	1.912339000000	H	-3.794948000000	-3.600601000000	2.572916000000
H	4.680834000000	2.992082000000	-2.185421000000	H	-5.081285000000	2.375340000000	-1.933522000000
H	3.331325000000	-0.689854000000	2.524635000000	H	-2.100470000000	5.310116000000	2.822925000000
H	0.735213000000	6.246126000000	2.582766000000	H	-2.786711000000	-1.706560000000	2.071439000000
H	-5.153152000000	1.787087000000	-2.164961000000	H	-0.107948000000	-4.164301000000	-2.616441000000
C	1.898934000000	-0.211376000000	-0.132178000000	C	-0.594368000000	-1.576639000000	-0.170127000000
O	1.680507000000	-0.728638000000	0.892576000000	O	-1.104266000000	-1.495099000000	0.879542000000
O	2.079247000000	0.317564000000	-1.159609000000	O	-0.070073000000	-1.626278000000	-1.211689000000
<b>PA[6]+3CO<sub>2</sub></b>				<b>PA[6]+4CO<sub>2</sub></b>			
O	-1.820397000000	-4.097060000000	2.094831000000	O	3.078218000000	4.394051000000	-2.523705000000
O	-4.777822000000	-3.204103000000	-2.515421000000	O	0.816385000000	4.660527000000	2.523400000000
O	-5.100998000000	2.487620000000	2.272074000000	O	-4.187128000000	3.410676000000	-2.513442000000
O	-5.098382000000	-0.440588000000	-2.430838000000	O	-1.986322000000	4.400828000000	2.470443000000

O	-2.631767000000	3.781469000000	2.227436000000	O	-4.733816000000	0.617015000000	-2.661897000000
O	-0.483242000000	5.141034000000	-2.695700000000	O	-5.390233000000	-1.939765000000	2.212249000000
C	-2.568437000000	-3.860470000000	0.937065000000	C	2.473040000000	4.493905000000	-1.276165000000
C	-2.244326000000	-4.539727000000	-0.246213000000	C	3.228590000000	4.102363000000	-0.163476000000
C	-3.011819000000	-4.276670000000	-1.379182000000	C	2.612571000000	4.162400000000	1.085349000000
H	-2.784015000000	-4.763946000000	-2.322547000000	H	3.151697000000	3.842825000000	1.972525000000
C	-4.082939000000	-3.378265000000	-1.352295000000	C	1.303823000000	4.630904000000	1.251067000000
C	-4.435873000000	-2.739578000000	-0.149523000000	C	0.581647000000	5.093046000000	0.134480000000
C	-3.646661000000	-2.982463000000	0.980970000000	C	1.185174000000	4.995151000000	-1.124991000000
H	-3.886002000000	-2.500600000000	1.926129000000	H	0.636391000000	5.334204000000	-2.002603000000
C	-5.669811000000	-1.857092000000	-0.047393000000	C	-0.791835000000	5.733474000000	0.271298000000
H	-6.363525000000	-2.111403000000	-0.856145000000	H	-0.855533000000	6.245289000000	1.237246000000
H	-6.189919000000	-2.092157000000	0.887764000000	H	-0.883260000000	6.512039000000	-0.494234000000
C	-5.375896000000	-0.370899000000	-0.069094000000	C	-1.974103000000	4.789576000000	0.124159000000
C	-5.073674000000	0.299429000000	-1.262278000000	C	-2.551915000000	4.155230000000	1.230691000000
C	-4.793354000000	1.661462000000	-1.271484000000	C	-3.670181000000	3.335902000000	1.089839000000
H	-4.560173000000	2.158943000000	-2.211206000000	H	-4.117355000000	2.878595000000	1.970718000000
C	-4.794523000000	2.414775000000	-0.093599000000	C	-4.246485000000	3.094836000000	-0.159716000000
C	-5.091871000000	1.747024000000	1.098037000000	C	-3.632468000000	3.680043000000	-1.273274000000
C	-5.382072000000	0.381778000000	1.105041000000	C	-2.532686000000	4.523774000000	-1.129001000000
H	-5.619119000000	-0.107193000000	2.047312000000	H	-2.096266000000	4.991160000000	-2.010028000000
C	-4.460743000000	3.895017000000	-0.125939000000	C	-5.501811000000	2.246925000000	-0.291346000000
H	-4.923511000000	4.335651000000	-1.015469000000	H	-6.169056000000	2.497076000000	0.540558000000
H	-4.924821000000	4.393209000000	0.732637000000	H	-6.034996000000	2.529654000000	-1.205289000000
C	-2.970360000000	4.194874000000	-0.167075000000	C	-5.256381000000	0.748555000000	-0.272982000000
C	-2.353711000000	4.510763000000	-1.381019000000	C	-5.385832000000	0.040173000000	0.924206000000
H	-2.929860000000	4.509113000000	-2.302697000000	H	-5.665836000000	0.557410000000	1.838342000000
C	-1.002430000000	4.850790000000	-1.458646000000	C	-5.193902000000	-1.341964000000	0.997082000000
C	-0.246284000000	4.952407000000	-0.277836000000	C	-4.870254000000	-2.056536000000	-0.173448000000
C	-0.841637000000	4.572141000000	0.925589000000	C	-4.718072000000	-1.344098000000	-1.364533000000
H	-0.272570000000	4.607215000000	1.850752000000	H	-4.454122000000	-1.865826000000	-2.280278000000
C	-2.174791000000	4.169301000000	0.992685000000	C	-4.893062000000	0.039845000000	-1.433551000000
C	1.153009000000	5.545311000000	-0.281525000000	C	-4.705188000000	-3.567556000000	-0.166270000000
H	1.294981000000	6.117107000000	-1.205186000000	H	-5.289227000000	-3.994581000000	0.656493000000
H	1.217164000000	6.268655000000	0.538855000000	H	-5.135753000000	-3.968669000000	-1.089675000000

H	-4.709279000000	0.073276000000	-3.154711000000	H	-2.328976000000	3.763590000000	3.116077000000
H	-3.578860000000	3.543831000000	2.204080000000	H	-4.634080000000	1.584627000000	-2.592183000000
H	-5.074918000000	-2.274819000000	-2.561301000000	H	-0.160019000000	4.609488000000	2.517372000000
H	-1.235530000000	-3.329134000000	2.225473000000	H	2.413701000000	4.535164000000	-3.215166000000
H	-4.934519000000	1.889916000000	3.019496000000	H	-3.597915000000	3.734780000000	-3.211803000000
H	0.444533000000	4.835820000000	-2.708617000000	H	-4.795105000000	-2.714790000000	2.277432000000
O	2.054620000000	3.888533000000	-2.404882000000	O	-3.222293000000	-3.626178000000	2.305963000000
O	4.577990000000	3.428365000000	2.510635000000	O	-0.725885000000	-5.401677000000	-2.314892000000
O	5.423420000000	-2.388336000000	-2.092586000000	O	4.137801000000	-2.655684000000	2.278784000000
O	4.860475000000	0.605083000000	2.533688000000	O	2.054156000000	-5.114516000000	-2.230673000000
O	2.696498000000	-3.039623000000	-2.122997000000	O	5.795217000000	-0.430337000000	2.163839000000
O	0.458884000000	-5.702970000000	2.193372000000	O	4.267962000000	1.838330000000	-2.657473000000
C	2.725655000000	3.767943000000	-1.195350000000	C	-2.570395000000	-4.053036000000	1.147109000000
C	2.287743000000	4.555732000000	-0.120790000000	C	-3.265624000000	-4.044344000000	-0.070409000000
C	2.938538000000	4.400200000000	1.101857000000	C	-2.585358000000	-4.492475000000	-1.202296000000
H	2.611786000000	4.968333000000	1.967972000000	H	-3.076700000000	-4.492171000000	-2.170744000000
C	4.014129000000	3.521207000000	1.264774000000	C	-1.267431000000	-4.963815000000	-1.144958000000
C	4.509885000000	2.818252000000	0.156785000000	C	-0.598547000000	-5.024418000000	0.093223000000
C	3.833174000000	2.937935000000	-1.063530000000	C	-1.272627000000	-4.547081000000	1.223157000000
H	4.191895000000	2.382273000000	-1.927316000000	H	-0.788509000000	-4.590740000000	2.196036000000
C	5.768868000000	1.972204000000	0.242697000000	C	0.773558000000	-5.666273000000	0.239955000000
H	6.336298000000	2.250224000000	1.136553000000	H	0.872984000000	-6.474307000000	-0.493113000000
H	6.409621000000	2.205184000000	-0.615408000000	H	0.821380000000	-6.141555000000	1.225630000000
C	5.482190000000	0.487357000000	0.243604000000	C	1.963117000000	-4.728769000000	0.116080000000
C	4.997209000000	-0.158492000000	1.388501000000	C	2.583527000000	-4.487192000000	-1.115770000000
C	4.685558000000	-1.514200000000	1.369296000000	C	3.712896000000	-3.675471000000	-1.211992000000
H	4.305229000000	-1.996444000000	2.268056000000	H	4.188848000000	-3.533964000000	-2.180553000000
C	4.829143000000	-2.277130000000	0.207263000000	C	4.256433000000	-3.046642000000	-0.088507000000
C	5.304348000000	-1.629788000000	-0.936828000000	C	3.611751000000	-3.252145000000	1.138196000000
C	5.631626000000	-0.275268000000	-0.914967000000	C	2.502483000000	-4.089952000000	1.235930000000
H	6.000393000000	0.204433000000	-1.819908000000	H	2.056949000000	-4.256316000000	2.213376000000
C	4.469782000000	-3.750073000000	0.193067000000	C	5.497756000000	-2.181411000000	-0.203275000000
H	4.851197000000	-4.209480000000	1.111110000000	H	6.010821000000	-2.439304000000	-1.136167000000
H	5.000867000000	-4.240936000000	-0.630837000000	H	6.191766000000	-2.428991000000	0.606979000000
C	2.981796000000	-4.051734000000	0.099047000000	C	5.225603000000	-0.686171000000	-0.198680000000



C	1.159063000000	4.754453000000	-0.768688000000	C	1.959070000000	4.753037000000	1.105707000000
C	1.586095000000	4.865115000000	0.560113000000	C	1.292866000000	4.971041000000	-0.106876000000
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H	0.900723000000	5.150573000000	2.584076000000	H	1.401020000000	4.610496000000	-2.225418000000
C	-0.746380000000	5.160144000000	1.228532000000	C	3.106342000000	3.784983000000	-1.245827000000
C	-1.164894000000	5.081870000000	-0.113642000000	C	3.786739000000	3.607355000000	-0.027150000000
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H	-0.474973000000	4.825518000000	-2.141725000000	H	3.699857000000	3.973627000000	2.091133000000
C	-2.622873000000	5.231770000000	-0.511481000000	C	5.161427000000	2.961621000000	0.045353000000
H	-3.079796000000	6.063479000000	0.036176000000	H	5.772352000000	3.301715000000	-0.798163000000
H	-2.665362000000	5.505605000000	-1.571073000000	H	5.664224000000	3.323908000000	0.949003000000
C	-3.450518000000	3.973797000000	-0.310039000000	C	5.155873000000	1.442349000000	0.080305000000
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C	-5.072774000000	2.666910000000	0.951604000000	C	5.365755000000	-0.713021000000	-1.028394000000
H	-5.737503000000	2.586039000000	1.810243000000	H	5.530126000000	-1.279414000000	-1.943409000000
C	-5.045304000000	1.632197000000	0.011367000000	C	5.189787000000	-1.405641000000	0.170399000000
C	-4.164892000000	1.772800000000	-1.072023000000	C	4.983947000000	-0.642561000000	1.327317000000
C	-3.407371000000	2.928842000000	-1.235355000000	C	4.974630000000	0.749216000000	1.280951000000
H	-2.771368000000	3.005832000000	-2.111069000000	H	4.831658000000	1.317063000000	2.199228000000
C	-5.979687000000	0.442342000000	0.150133000000	C	5.205740000000	-2.921671000000	0.207279000000
H	-6.599257000000	0.594918000000	1.040755000000	H	5.821094000000	-3.278969000000	-0.625921000000
H	-6.666285000000	0.427798000000	-0.704636000000	H	5.697057000000	-3.263653000000	1.124187000000
C	-5.297319000000	-0.906907000000	0.247876000000	C	3.830329000000	-3.562641000000	0.099484000000
C	-4.756476000000	-1.344949000000	1.459594000000	C	3.237971000000	-3.734905000000	-1.153703000000
H	-4.816327000000	-0.717491000000	2.345116000000	H	3.736368000000	-3.371026000000	-2.048517000000
C	-4.130276000000	-2.589616000000	1.580343000000	C	2.016954000000	-4.391994000000	-1.313398000000
C	-4.037504000000	-3.428868000000	0.451980000000	C	1.369640000000	-4.932495000000	-0.185582000000
C	-4.575109000000	-2.985440000000	-0.756434000000	C	1.936608000000	-4.712734000000	1.071650000000
H	-4.512442000000	-3.607706000000	-1.644441000000	H	1.450088000000	-5.097514000000	1.963876000000
C	-5.198756000000	-1.745309000000	-0.876953000000	C	3.139084000000	-4.023198000000	1.234235000000
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H	-3.511238000000	-5.256400000000	1.469791000000	H	0.106179000000	-6.291637000000	-1.271999000000
H	-3.747270000000	-5.418562000000	-0.260579000000	H	0.126031000000	-6.539339000000	0.464295000000
H	-4.838264000000	4.569757000000	2.496916000000	H	5.521264000000	0.741559000000	-3.008106000000
H	-5.408858000000	-0.500030000000	-2.303125000000	H	4.117800000000	-3.052779000000	2.578353000000

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H	-3.351633000000	0.191341000000	-1.863442000000	H	4.572972000000	-0.710358000000	3.221859000000
H	-2.948367000000	-3.599802000000	2.750632000000	H	0.575300000000	-4.626995000000	-2.582524000000
O	-1.427636000000	-4.734424000000	2.619790000000	O	-1.263259000000	-4.608907000000	-2.513920000000
O	0.452623000000	-4.283094000000	-2.567902000000	O	-3.460952000000	-3.992031000000	2.535220000000
O	5.251641000000	-2.199715000000	2.500691000000	O	-5.610179000000	1.306995000000	-2.162946000000
O	2.995147000000	-3.043057000000	-2.489541000000	O	-4.553112000000	-1.405851000000	2.547729000000
O	3.847975000000	0.264321000000	2.552854000000	O	-3.555970000000	3.241499000000	-2.380880000000
O	4.798100000000	4.079148000000	-1.354932000000	O	-1.430118000000	5.141025000000	2.376517000000
C	-0.914303000000	-4.702304000000	1.329170000000	C	-1.846505000000	-4.428205000000	-1.265217000000
C	-1.828847000000	-4.654637000000	0.270231000000	C	-1.191653000000	-4.987421000000	-0.159529000000
C	-1.318871000000	-4.492204000000	-1.018846000000	C	-1.771056000000	-4.796291000000	1.093441000000
H	-1.995808000000	-4.384319000000	-1.861082000000	H	-1.287342000000	-5.192700000000	1.981304000000
C	0.056080000000	-4.470625000000	-1.271987000000	C	-2.973410000000	-4.101863000000	1.261467000000
C	0.961044000000	-4.699004000000	-0.220575000000	C	-3.658841000000	-3.610253000000	0.137607000000
C	0.454164000000	-4.762833000000	1.082437000000	C	-3.060360000000	-3.765344000000	-1.118952000000
H	1.142130000000	-4.892321000000	1.915786000000	H	-3.575372000000	-3.386729000000	-2.001432000000
C	2.434565000000	-4.968781000000	-0.483217000000	C	-5.042982000000	-2.990553000000	0.252009000000
H	2.554397000000	-5.339536000000	-1.506074000000	H	-5.521331000000	-3.351110000000	1.168834000000
H	2.751916000000	-5.784259000000	0.176435000000	H	-5.656185000000	-3.357740000000	-0.578906000000
C	3.350087000000	-3.786863000000	-0.253840000000	C	-5.064753000000	-1.475080000000	0.224968000000
C	3.604252000000	-2.848702000000	-1.262562000000	C	-4.802956000000	-0.716349000000	1.372661000000
C	4.464861000000	-1.777682000000	-1.034421000000	C	-4.831380000000	0.675043000000	1.338708000000
H	4.687983000000	-1.084774000000	-1.839252000000	H	-4.632805000000	1.242366000000	2.246517000000
C	5.037071000000	-1.555664000000	0.220187000000	C	-5.108057000000	1.371005000000	0.158809000000
C	4.742405000000	-2.465844000000	1.238490000000	C	-5.348927000000	0.613665000000	-0.991066000000
C	3.943924000000	-3.580491000000	0.991546000000	C	-5.338040000000	-0.779232000000	-0.953520000000
H	3.745848000000	-4.285944000000	1.795904000000	H	-5.549074000000	-1.341940000000	-1.861602000000
C	5.894168000000	-0.328574000000	0.468266000000	C	-5.128977000000	2.889368000000	0.136091000000
H	6.619571000000	-0.232656000000	-0.346965000000	H	-5.613796000000	3.241184000000	1.053154000000
H	6.482559000000	-0.471136000000	1.381720000000	H	-5.759497000000	3.231543000000	-0.691876000000
C	5.088415000000	0.957420000000	0.550210000000	C	-3.755176000000	3.535110000000	0.047662000000
C	5.258285000000	1.954749000000	-0.414392000000	C	-3.141522000000	4.019107000000	1.206249000000
H	5.956213000000	1.807639000000	-1.234753000000	H	-3.634680000000	3.911378000000	2.169019000000

C	4.564047000000	3.165750000000	-0.359606000000	C	-1.911897000000	4.679712000000	1.180290000000
C	3.695141000000	3.420098000000	0.716115000000	C	-1.275294000000	4.901824000000	-0.055111000000
C	3.482652000000	2.403448000000	1.649201000000	C	-1.863921000000	4.374611000000	-1.206525000000
H	2.798613000000	2.560923000000	2.478517000000	H	-1.389824000000	4.518127000000	-2.173631000000
C	4.155775000000	1.185047000000	1.579841000000	C	-3.078788000000	3.687880000000	-1.176571000000
C	3.055221000000	4.782808000000	0.919924000000	C	-0.013141000000	5.743629000000	-0.168130000000
H	3.615291000000	5.530397000000	0.346677000000	H	-0.018924000000	6.510941000000	0.613940000000
H	3.166746000000	5.060932000000	1.973569000000	H	-0.045447000000	6.277189000000	-1.124001000000
H	2.968845000000	-2.197819000000	-2.968714000000	H	-4.262353000000	-0.786904000000	3.234574000000
H	4.517437000000	-0.442165000000	2.614596000000	H	-4.329717000000	2.659027000000	-2.266684000000
H	1.358958000000	-3.910534000000	-2.581182000000	H	-3.936636000000	-3.143000000000	2.618568000000
H	-0.730987000000	-4.471743000000	3.241311000000	H	-1.716586000000	-4.051700000000	-3.164323000000
H	4.808186000000	-2.772105000000	3.146695000000	H	-5.628601000000	0.688176000000	-2.908945000000
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C	-1.600060000000	-1.105564000000	0.862003000000	C	-1.882411000000	0.280639000000	-1.264746000000
O	-1.960428000000	-0.640669000000	-0.150764000000	H	-2.342888000000	0.928905000000	-2.014922000000
O	-1.201017000000	-1.550215000000	1.863408000000	H	-0.794023000000	0.340591000000	-1.351381000000
C	1.692471000000	-1.399689000000	1.690042000000	H	-2.187672000000	0.622391000000	-0.272807000000
O	1.549578000000	-0.829834000000	0.679299000000	H	-2.206913000000	-0.755253000000	-1.401364000000
O	1.805407000000	-1.999763000000	2.687785000000				
C	-0.394366000000	1.716139000000	-0.484734000000				
O	-0.561693000000	1.621933000000	-1.641018000000				
O	-0.235077000000	1.789471000000	0.667892000000				
C	2.612898000000	0.756821000000	-2.611333000000				
O	2.960566000000	-0.112323000000	-3.313256000000				
O	2.277030000000	1.643541000000	-1.933709000000				
C	-0.656190000000	-1.435020000000	-2.566678000000				
O	-1.762360000000	-1.571249000000	-2.914072000000				
O	0.451402000000	-1.279676000000	-2.221898000000				
<b>PA[6]+2CH<sub>4</sub></b>				<b>PA[6]+3CH<sub>4</sub></b>			
O	1.141664000000	-4.261799000000	-2.551632000000	O	-2.436651000000	-4.396226000000	-2.664254000000
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O	5.971503000000	1.294889000000	-1.919493000000	O	4.880837000000	-3.236599000000	-2.191997000000
O	4.369372000000	-1.598072000000	2.522814000000	O	2.153302000000	-4.070385000000	2.556107000000
O	3.885802000000	3.185468000000	-2.262143000000	O	5.146176000000	-0.417967000000	-2.524687000000

O	1.397198000000	5.036462000000	2.335250000000	O	4.776451000000	2.505516000000	2.173139000000
C	1.778036000000	-4.248794000000	-1.316298000000	C	-1.915836000000	-4.553137000000	-1.384094000000
C	1.147394000000	-4.915681000000	-0.256984000000	C	-2.790950000000	-4.352930000000	-0.309527000000
C	1.776458000000	-4.884533000000	0.986399000000	C	-2.266009000000	-4.452894000000	0.977135000000
H	1.312044000000	-5.365326000000	1.842419000000	H	-2.901432000000	-4.269857000000	1.838450000000
C	3.004355000000	-4.245954000000	1.183343000000	C	-0.927455000000	-4.781723000000	1.210578000000
C	3.666585000000	-3.653336000000	0.095660000000	C	-0.080805000000	-5.075220000000	0.126407000000
C	3.018761000000	-3.644204000000	-1.145578000000	C	-0.593494000000	-4.926374000000	-1.167986000000
H	3.510181000000	-3.174649000000	-1.997015000000	H	0.051542000000	-5.134942000000	-2.021116000000
C	5.072385000000	-3.088774000000	0.228430000000	C	1.325752000000	-5.616932000000	0.330855000000
H	5.541928000000	-3.508121000000	1.124680000000	H	1.372670000000	-6.131455000000	1.296771000000
H	5.670116000000	-3.435865000000	-0.622272000000	H	1.511059000000	-6.382317000000	-0.431377000000
C	5.136089000000	-1.576177000000	0.271440000000	C	2.442185000000	-4.592987000000	0.251724000000
C	4.754708000000	-0.862659000000	1.415313000000	C	2.831922000000	-3.844634000000	1.369054000000
C	4.794742000000	0.527809000000	1.442135000000	C	3.890728000000	-2.943737000000	1.300422000000
H	4.495097000000	1.060723000000	2.342910000000	H	4.184519000000	-2.386589000000	2.188279000000
C	5.208900000000	1.267468000000	0.330755000000	C	4.597410000000	-2.737435000000	0.113336000000
C	5.578378000000	0.555857000000	-0.813769000000	C	4.185230000000	-3.456344000000	-1.013333000000
C	5.552069000000	-0.837587000000	-0.837118000000	C	3.137687000000	-4.373185000000	-0.939508000000
H	5.854996000000	-1.365920000000	-1.739859000000	H	2.861602000000	-4.944909000000	-1.824324000000
C	5.240329000000	2.785227000000	0.373732000000	C	5.762055000000	-1.764274000000	0.061094000000
H	5.635293000000	3.095351000000	1.347208000000	H	6.338572000000	-1.867620000000	0.986771000000
H	5.950583000000	3.155323000000	-0.373794000000	H	6.437379000000	-2.045296000000	-0.753948000000
C	3.883804000000	3.442889000000	0.179522000000	C	5.339992000000	-0.312662000000	-0.082659000000
C	3.180945000000	3.919657000000	1.289208000000	C	5.218060000000	0.488882000000	1.054351000000
H	3.597580000000	3.805741000000	2.286731000000	H	5.417250000000	0.072534000000	2.038443000000
C	1.958561000000	4.584525000000	1.172858000000	C	4.863299000000	1.836167000000	0.982677000000
C	1.415664000000	4.807599000000	-0.107004000000	C	4.648164000000	2.426382000000	-0.276539000000
C	2.098919000000	4.295050000000	-1.212520000000	C	4.738915000000	1.615816000000	-1.410889000000
H	1.703663000000	4.447635000000	-2.213060000000	H	4.569653000000	2.040568000000	-2.396559000000
C	3.311301000000	3.613624000000	-1.093747000000	C	5.063273000000	0.259534000000	-1.337508000000
C	0.160418000000	5.640691000000	-0.315907000000	C	4.341810000000	3.907269000000	-0.431127000000
H	0.164831000000	6.485501000000	0.382514000000	H	4.947829000000	4.486636000000	0.274457000000
H	0.207131000000	6.075159000000	-1.319995000000	H	4.657489000000	4.218165000000	-1.432622000000
H	3.981411000000	-1.009796000000	3.188083000000	H	2.421609000000	-3.412979000000	3.216018000000



H	4.669172000000	2.629068000000	-2.096302000000	H	5.144721000000	-1.382573000000	-2.383286000000
H	3.977686000000	-3.422009000000	2.605230000000	H	0.425463000000	-4.659927000000	2.579649000000
H	1.574923000000	-3.628306000000	-3.143377000000	H	-1.714463000000	-4.425177000000	-3.309944000000
H	6.077050000000	0.705441000000	-2.681911000000	H	4.438921000000	-3.696497000000	-2.921939000000
H	0.460344000000	5.280655000000	2.205810000000	H	4.328694000000	3.367436000000	2.066834000000
O	-1.341618000000	5.575710000000	2.088153000000	O	3.275607000000	4.856689000000	2.018774000000
O	-3.386615000000	3.001346000000	-2.367558000000	O	-0.118307000000	4.404798000000	-2.334725000000
O	-4.654229000000	-1.221466000000	2.631195000000	O	-3.969027000000	1.959640000000	2.336442000000
O	-5.683726000000	1.400693000000	-2.137552000000	O	-2.849431000000	5.085945000000	-2.099264000000
O	-3.561677000000	-3.850790000000	2.591801000000	O	-5.668524000000	-0.288882000000	2.303069000000
O	-1.671365000000	-4.275900000000	-2.605618000000	O	-3.955968000000	-1.987958000000	-2.690555000000
C	-1.888132000000	4.895123000000	1.005030000000	C	2.380160000000	4.748797000000	0.959293000000
C	-1.159485000000	4.897285000000	-0.190466000000	C	2.877739000000	4.276999000000	-0.260240000000
C	-1.711696000000	4.223939000000	-1.278459000000	C	1.980731000000	4.168372000000	-1.321191000000
H	-1.180038000000	4.196770000000	-2.225025000000	H	2.323569000000	3.802638000000	-2.284539000000
C	-2.957575000000	3.590350000000	-1.214442000000	C	0.636434000000	4.536910000000	-1.205755000000
C	-3.696867000000	3.622480000000	-0.017139000000	C	0.151076000000	5.031471000000	0.019822000000
C	-3.129853000000	4.274385000000	1.084749000000	C	1.047619000000	5.120706000000	1.091404000000
H	-3.692456000000	4.321417000000	2.016852000000	H	0.692682000000	5.510716000000	2.044739000000
C	-5.090833000000	3.026414000000	0.095831000000	C	-1.272263000000	5.532590000000	0.192032000000
H	-5.707916000000	3.362592000000	-0.744998000000	H	-1.487051000000	6.297758000000	-0.563115000000
H	-5.564563000000	3.431526000000	0.996953000000	H	-1.338465000000	6.042614000000	1.159482000000
C	-5.135260000000	1.509904000000	0.172124000000	C	-2.361897000000	4.475099000000	0.142901000000
C	-5.444264000000	0.731030000000	-0.945670000000	C	-3.162186000000	4.311672000000	-0.991289000000
C	-5.507756000000	-0.657930000000	-0.863746000000	C	-4.230144000000	3.417842000000	-1.002190000000
H	-5.757520000000	-1.238300000000	-1.750007000000	H	-4.848833000000	3.328438000000	-1.893433000000
C	-5.239314000000	-1.329510000000	0.328514000000	C	-4.519391000000	2.621290000000	0.106265000000
C	-4.907972000000	-0.551614000000	1.446323000000	C	-3.684585000000	2.742513000000	1.225183000000
C	-4.867038000000	0.838177000000	1.368873000000	C	-2.639293000000	3.662754000000	1.246291000000
H	-4.616722000000	1.421606000000	2.253658000000	H	-2.033780000000	3.761814000000	2.144520000000
C	-5.249824000000	-2.842817000000	0.389085000000	C	-5.670492000000	1.638196000000	0.078182000000
H	-5.911501000000	-3.216587000000	-0.400289000000	H	-6.316301000000	1.887767000000	-0.771341000000
H	-5.678269000000	-3.177993000000	1.339013000000	H	-6.284860000000	1.756526000000	0.976918000000
C	-3.873686000000	-3.463433000000	0.202344000000	C	-5.233571000000	0.189221000000	-0.048670000000
C	-3.328258000000	-3.576044000000	-1.078153000000	C	-4.767285000000	-0.295698000000	-1.272577000000



O	0.554234000000	4.342463000000	-2.729788000000	O	-1.648363000000	-3.974648000000	-2.625177000000
O	-0.864345000000	4.918389000000	2.597293000000	O	1.042880000000	-5.488921000000	1.977889000000
C	4.564896000000	-3.231324000000	-0.644633000000	C	-3.861647000000	3.164205000000	-1.421268000000
C	3.769085000000	-3.513327000000	0.470826000000	C	-3.371149000000	3.880026000000	-0.321750000000
C	3.720482000000	-2.559978000000	1.488026000000	C	-3.667157000000	3.390201000000	0.949079000000
H	3.109439000000	-2.738150000000	2.367934000000	H	-3.281200000000	3.897005000000	1.828652000000
C	4.443402000000	-1.364823000000	1.422273000000	C	-4.460860000000	2.254963000000	1.142640000000
C	5.242794000000	-1.094860000000	0.295720000000	C	-5.019832000000	1.595394000000	0.033601000000
C	5.285623000000	-2.046191000000	-0.727870000000	C	-4.680783000000	2.054921000000	-1.244396000000
H	5.903214000000	-1.852637000000	-1.604147000000	H	-5.089527000000	1.545231000000	-2.116205000000
C	6.022046000000	0.197494000000	0.158840000000	C	-5.991625000000	0.434377000000	0.187102000000
H	6.649143000000	0.365556000000	1.041081000000	H	-6.531627000000	0.529106000000	1.134755000000
H	6.711116000000	0.103747000000	-0.687953000000	H	-6.745740000000	0.505946000000	-0.604607000000
C	5.133877000000	1.408346000000	-0.069444000000	C	-5.325875000000	-0.924966000000	0.099406000000
C	4.915418000000	2.351875000000	0.937095000000	C	-4.755828000000	-1.536257000000	1.222328000000
C	4.153956000000	3.493464000000	0.698644000000	C	-4.085475000000	-2.752781000000	1.118265000000
H	4.028968000000	4.232412000000	1.487798000000	H	-3.653294000000	-3.208412000000	2.006979000000
C	3.526434000000	3.704264000000	-0.529623000000	C	-3.959140000000	-3.412523000000	-0.106931000000
C	3.675805000000	2.714341000000	-1.509930000000	C	-4.534196000000	-2.802232000000	-1.226876000000
C	4.485273000000	1.603513000000	-1.291364000000	C	-5.207669000000	-1.588006000000	-1.123091000000
H	4.608076000000	0.859631000000	-2.076231000000	H	-5.644785000000	-1.137887000000	-2.013058000000
C	2.688985000000	4.943346000000	-0.770434000000	C	-3.249104000000	-4.751390000000	-0.206393000000
H	3.100095000000	5.757169000000	-0.162571000000	H	-3.522041000000	-5.346858000000	0.671363000000
H	2.786793000000	5.258302000000	-1.814383000000	H	-3.638922000000	-5.298038000000	-1.072724000000
C	1.217969000000	4.784922000000	-0.421118000000	C	-1.729896000000	-4.693091000000	-0.277088000000
C	0.801663000000	4.890097000000	0.908499000000	C	-0.974153000000	-5.037270000000	0.847059000000
H	1.532175000000	5.013851000000	1.703591000000	H	-1.470413000000	-5.283403000000	1.782241000000
C	-0.545528000000	4.841149000000	1.262959000000	C	0.419029000000	-5.118872000000	0.815920000000
C	-1.523799000000	4.771459000000	0.255246000000	C	1.097943000000	-4.883169000000	-0.393274000000
C	-1.106555000000	4.590489000000	-1.063908000000	C	0.348897000000	-4.476143000000	-1.499634000000
H	-1.840249000000	4.472062000000	-1.856411000000	H	0.843762000000	-4.268645000000	-2.444406000000
C	0.244912000000	4.553341000000	-1.409081000000	C	-1.042344000000	-4.365990000000	-1.461118000000
C	-3.003648000000	4.909422000000	0.572532000000				
H	-3.123000000000	5.339065000000	1.572552000000				
H	-3.443340000000	5.627806000000	-0.128196000000				

H	5.151825000000	2.736694000000	2.821132000000	C	2.594717000000	-5.122981000000	-0.538997000000
H	1.424051000000	3.903329000000	-2.787082000000	H	2.899752000000	-5.929666000000	0.136912000000
H	4.846505000000	0.293111000000	2.386232000000	H	2.781177000000	-5.486695000000	-1.554998000000
H	5.103516000000	-3.830566000000	-2.410377000000	H	-4.286755000000	-1.259492000000	3.084363000000
H	3.037355000000	2.079551000000	-3.225474000000	H	-2.616998000000	-3.917760000000	-2.529884000000
H	-1.634146000000	4.336660000000	2.747261000000	H	-4.897573000000	0.922317000000	2.472113000000
O	-2.893453000000	2.919531000000	2.571983000000	H	-3.801438000000	2.987812000000	-3.353262000000
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O	-4.355968000000	-4.589499000000	1.561481000000	H	1.977983000000	-5.204666000000	1.962130000000
O	-4.438696000000	-0.523854000000	-2.200431000000	O	3.629378000000	-4.439391000000	2.015183000000
O	-1.625717000000	-4.967029000000	2.067138000000	O	4.907244000000	-1.212060000000	-2.299538000000
O	1.882167000000	-4.507673000000	-2.201214000000	O	2.947686000000	3.064300000000	2.263177000000
C	-3.680608000000	2.631456000000	1.465706000000	O	6.159830000000	1.275673000000	-1.887262000000
C	-3.769789000000	3.609680000000	0.465676000000	O	1.477145000000	5.450028000000	2.247043000000
C	-4.530902000000	3.314736000000	-0.664023000000	O	-0.750554000000	4.190318000000	-2.672420000000
H	-4.595081000000	4.028867000000	-1.479717000000	C	3.953669000000	-3.583953000000	0.967177000000
C	-5.199911000000	2.096864000000	-0.804844000000	C	3.470532000000	-3.905635000000	-0.305798000000
C	-5.167344000000	1.155456000000	0.235312000000	C	3.819602000000	-3.060546000000	-1.357693000000
C	-4.381355000000	1.434425000000	1.359969000000	H	3.474492000000	-3.275814000000	-2.364618000000
H	-4.323913000000	0.700891000000	2.163034000000	C	4.620744000000	-1.928579000000	-1.174444000000
C	-5.983104000000	-0.121786000000	0.159460000000	C	5.089017000000	-1.606548000000	0.112837000000
H	-6.738348000000	-0.011835000000	-0.626587000000	C	4.742504000000	-2.457812000000	1.168525000000
H	-6.535585000000	-0.246885000000	1.097991000000	H	5.110857000000	-2.234622000000	2.169105000000
C	-5.160233000000	-1.370174000000	-0.081458000000	C	5.959794000000	-0.391332000000	0.379980000000
C	-4.373607000000	-1.517364000000	-1.231608000000	H	6.821196000000	-0.386498000000	-0.297553000000
C	-3.594889000000	-2.654819000000	-1.428733000000	H	6.372668000000	-0.477635000000	1.391067000000
H	-3.000751000000	-2.740752000000	-2.335396000000	C	5.230752000000	0.937598000000	0.272044000000
C	-3.572323000000	-3.695513000000	-0.496337000000	C	5.366898000000	1.753801000000	-0.854906000000
C	-4.369193000000	-3.550531000000	0.644197000000	C	4.739463000000	2.995008000000	-0.934728000000
C	-5.145014000000	-2.411740000000	0.847967000000	H	4.885251000000	3.614648000000	-1.817951000000
H	-5.747886000000	-2.326339000000	1.750777000000	C	3.922295000000	3.461156000000	0.096621000000
C	-2.729104000000	-4.937705000000	-0.724922000000	C	3.744790000000	2.624735000000	1.206674000000
H	-2.789912000000	-5.202872000000	-1.785752000000				
H	-3.171398000000	-5.778194000000	-0.177836000000				
C	-1.259747000000	-4.797043000000	-0.357102000000				

C	-0.304849000000	-4.661634000000	-1.368514000000	C	4.399645000000	1.398945000000	1.296934000000
H	-0.617894000000	-4.620143000000	-2.408448000000	H	4.261342000000	0.795343000000	2.190363000000
C	1.065918000000	-4.621809000000	-1.107641000000	C	3.268483000000	4.825139000000	0.011235000000
C	1.519110000000	-4.730052000000	0.220974000000	H	3.670586000000	5.343386000000	-0.866731000000
C	0.562442000000	-4.824880000000	1.234039000000	H	3.561699000000	5.424112000000	0.880623000000
H	0.877309000000	-4.908726000000	2.270504000000	C	1.753911000000	4.807724000000	-0.087256000000
C	-0.808577000000	-4.853753000000	0.973895000000	C	1.128979000000	4.470433000000	-1.290236000000
C	2.995419000000	-4.815818000000	0.577399000000	H	1.722854000000	4.165303000000	-2.147709000000
H	3.482331000000	-5.574725000000	-0.046276000000	C	-0.258577000000	4.529030000000	-1.443642000000
H	3.073182000000	-5.176794000000	1.608167000000	C	-1.055524000000	4.975521000000	-0.370164000000
H	-3.541569000000	-0.283983000000	-2.482866000000	C	-0.429372000000	5.265804000000	0.843947000000
H	-2.568885000000	-4.953603000000	1.819511000000	H	-1.020068000000	5.579676000000	1.700320000000
H	-5.652719000000	0.967802000000	-2.260681000000	C	0.951216000000	5.163816000000	1.008885000000
H	-2.723026000000	2.103327000000	3.065689000000	C	-2.558082000000	5.151507000000	-0.502526000000
H	-4.860184000000	-4.333745000000	2.349265000000	H	-2.796714000000	5.599547000000	-1.473520000000
H	2.827306000000	-4.512779000000	-1.956257000000	H	-2.884035000000	5.872475000000	0.254562000000
C	1.397655000000	1.262638000000	1.390933000000	H	6.085579000000	1.868178000000	-2.651629000000
H	1.701193000000	1.543034000000	0.379851000000	H	2.181228000000	4.793678000000	2.417160000000
H	2.262139000000	0.874749000000	1.936422000000	H	5.449195000000	-0.422105000000	-2.112367000000
H	0.991096000000	2.145195000000	1.892847000000	H	3.878340000000	-4.026614000000	2.855879000000
H	0.633519000000	0.483490000000	1.335073000000	H	2.171053000000	2.484192000000	2.332375000000
C	-1.434983000000	1.107693000000	-1.439175000000	H	-1.721217000000	4.084740000000	-2.656526000000
H	-2.479754000000	1.425132000000	-1.383030000000	C	-1.598715000000	-0.715976000000	-0.916875000000
H	-1.356946000000	0.061762000000	-1.757505000000	H	-0.913602000000	-1.089733000000	-0.152142000000
H	-0.894232000000	1.751906000000	-2.137231000000	H	-1.702383000000	-1.475549000000	-1.696424000000
H	-0.989655000000	1.203810000000	-0.446674000000	H	-2.573186000000	-0.511677000000	-0.466575000000
C	1.745121000000	-1.022279000000	-1.488457000000	H	-1.193733000000	0.205918000000	-1.342389000000
H	1.768652000000	-0.132595000000	-2.127546000000	C	1.958439000000	0.513929000000	-1.584372000000
H	2.476527000000	-0.913214000000	-0.685283000000	H	2.787925000000	0.229750000000	-2.236485000000
H	0.747708000000	-1.118562000000	-1.052904000000	H	2.354635000000	0.825963000000	-0.615603000000
H	1.966648000000	-1.919607000000	-2.071592000000	H	1.391658000000	1.340312000000	-2.023594000000
C	-1.579420000000	-1.428320000000	1.570791000000	H	1.300562000000	-0.347536000000	-1.444105000000
H	-2.410796000000	-1.069059000000	0.959314000000				
H	-0.709056000000	-1.607586000000	0.934411000000				
H	-1.324652000000	-0.677494000000	2.325675000000				

H	-1.851669000000	-2.367219000000	2.058590000000	C	-1.998893000000	-0.203342000000	3.384961000000
				H	-0.978098000000	0.108070000000	3.616513000000
				H	-1.994089000000	-0.750393000000	2.437721000000
				H	-2.354313000000	-0.850195000000	4.196403000000
				H	-2.637472000000	0.678445000000	3.294759000000
				C	1.255454000000	-1.856947000000	1.803310000000
				H	0.302323000000	-1.412870000000	2.096810000000
				H	1.391058000000	-2.803323000000	2.331821000000
				H	1.255603000000	-2.050122000000	0.728782000000
				H	2.075604000000	-1.172725000000	2.040365000000
				C	-0.005934000000	1.815292000000	1.307606000000
				H	0.386173000000	2.344196000000	0.437359000000
				H	-0.064300000000	2.503810000000	2.156563000000
				H	-1.012864000000	1.454868000000	1.085924000000
				H	0.628341000000	0.953580000000	1.538890000000
<b>PA[6]+1-n-butane (along z-axis)</b>				<b>PA[6]+1-n-butane (along x-axis)</b>			
O	2.539228000000	-5.084776000000	-2.239606000000	O	1.637158000000	-3.890090000000	-2.528134000000
O	3.825637000000	-2.652968000000	2.568176000000	O	4.025857000000	-3.892220000000	2.473136000000
O	4.741099000000	1.925432000000	-2.496992000000	O	5.823312000000	1.873202000000	-1.933456000000
O	5.491152000000	-0.381386000000	2.483392000000	O	4.626467000000	-1.119073000000	2.571881000000
O	2.840050000000	4.026466000000	-2.565384000000	O	3.332010000000	3.186263000000	-2.223016000000
O	0.930729000000	5.036883000000	2.543644000000	O	0.961439000000	5.381229000000	2.283722000000
C	2.908947000000	-4.451429000000	-1.056891000000	C	2.280641000000	-3.893276000000	-1.295190000000
C	2.140841000000	-4.722760000000	0.081060000000	C	1.707122000000	-4.650015000000	-0.264897000000
C	2.486306000000	-4.071433000000	1.263987000000	C	2.327204000000	-4.610637000000	0.983327000000
H	1.905441000000	-4.242844000000	2.165587000000	C	1.898245000000	-5.153742000000	1.820392000000
C	3.578334000000	-3.200136000000	1.344684000000	C	3.498336000000	-3.881103000000	1.207508000000
C	4.377293000000	-2.978528000000	0.206498000000	C	4.121389000000	-3.217522000000	0.138858000000
C	4.009805000000	-3.605256000000	-0.989456000000	C	3.475123000000	-3.210208000000	-1.102160000000
H	4.618215000000	-3.445507000000	-1.879202000000	H	3.926633000000	-2.669039000000	-1.932556000000
C	5.624092000000	-2.111921000000	0.250343000000	C	5.474919000000	-2.543962000000	0.294358000000
H	6.179201000000	-2.304995000000	1.174704000000	H	5.961952000000	-2.912954000000	1.202532000000
H	6.284766000000	-2.415896000000	-0.569195000000				
C	5.358066000000	-0.621972000000	0.122560000000				

C	5.305777000000	0.212617000000	1.242956000000	H	6.115745000000	-2.842519000000	-0.543324000000
C	5.099225000000	1.584031000000	1.111720000000	C	5.383055000000	-1.034609000000	0.320114000000
H	5.082187000000	2.213573000000	1.999628000000	C	4.917714000000	-0.356088000000	1.453923000000
C	4.911735000000	2.176442000000	-0.138285000000	C	4.774421000000	1.027766000000	1.452962000000
C	4.927810000000	1.335026000000	-1.257996000000	H	4.408265000000	1.536188000000	2.343331000000
C	5.156390000000	-0.032389000000	-1.128108000000	C	5.077811000000	1.790710000000	0.321315000000
H	5.183820000000	-0.661277000000	-2.016600000000	C	5.534499000000	1.111088000000	-0.811285000000
C	4.679676000000	3.670365000000	-0.265364000000	C	5.691881000000	-0.273355000000	-0.807009000000
H	5.245200000000	4.174211000000	0.526220000000	H	6.055270000000	-0.777157000000	-1.701484000000
H	5.091406000000	4.027044000000	-1.215156000000	C	4.905450000000	3.298754000000	0.327344000000
C	3.221080000000	4.083714000000	-0.150418000000	H	5.283582000000	3.686844000000	1.279278000000
C	2.666715000000	4.331221000000	1.107457000000	H	5.539974000000	3.737764000000	-0.450881000000
H	3.263886000000	4.191889000000	2.005009000000	C	3.469866000000	3.770214000000	0.159963000000
C	1.359339000000	4.792507000000	1.264885000000	C	2.789933000000	4.311738000000	1.254058000000
C	0.578073000000	5.055381000000	0.124059000000	H	3.276898000000	4.365591000000	2.224331000000
C	1.110625000000	4.747970000000	-1.130158000000	C	1.499351000000	4.834237000000	1.149696000000
H	0.523668000000	4.918832000000	-2.028473000000	C	0.859971000000	4.844290000000	-0.103701000000
C	2.406499000000	4.251617000000	-1.285283000000	C	1.517140000000	4.253227000000	-1.185415000000
C	-0.790850000000	5.709230000000	0.226645000000	H	1.046482000000	4.237395000000	-2.164609000000
H	-0.833621000000	6.319755000000	1.135196000000	C	2.799757000000	3.713755000000	-1.076848000000
H	-0.903486000000	6.399600000000	-0.616033000000	C	-0.467416000000	5.554127000000	-0.321902000000
H	5.318512000000	0.268041000000	3.182608000000	H	-0.528551000000	6.415805000000	0.352538000000
H	3.540189000000	3.347281000000	-2.566011000000	H	-0.469756000000	5.959727000000	-1.339163000000
H	4.472121000000	-1.922307000000	2.519536000000	H	4.162414000000	-0.574680000000	3.225711000000
H	3.064626000000	-4.728797000000	-2.972270000000	H	4.242621000000	2.865542000000	-2.089382000000
H	4.635872000000	1.239371000000	-3.173626000000	H	4.385932000000	-3.002579000000	2.651154000000
H	-0.039005000000	4.927575000000	2.587326000000	H	1.989998000000	-3.168557000000	-3.070645000000
O	-1.828993000000	4.502178000000	2.573211000000	H	6.016116000000	1.286361000000	-2.680795000000
O	-4.217722000000	3.294661000000	-2.271558000000	H	-0.013405000000	5.399182000000	2.223074000000
O	-4.766355000000	-2.300945000000	2.186344000000	O	-1.832828000000	5.293455000000	2.149783000000
O	-5.011690000000	0.732387000000	-2.314290000000	O	-3.890160000000	2.696393000000	-2.287289000000
O	-3.270610000000	-4.728688000000	2.212032000000	O	-4.403942000000	-1.730842000000	2.697278000000
O	-0.194850000000	-4.424803000000	-2.391457000000				
C	-2.451040000000	4.157590000000	1.379346000000				
C	-1.961438000000	4.745081000000	0.202826000000				

C	-2.584097000000	4.406037000000	-0.993942000000	O	-5.946868000000	0.817406000000	-1.973255000000
H	-2.225446000000	4.821042000000	-1.931006000000	O	-3.117936000000	-4.286052000000	2.620005000000
C	-3.677869000000	3.531584000000	-1.050775000000	O	-1.159901000000	-4.123881000000	-2.566807000000
C	-4.194802000000	2.997483000000	0.144555000000	C	-2.372410000000	4.598719000000	1.073120000000
C	-3.549516000000	3.308448000000	1.348696000000	C	-1.712701000000	4.701474000000	-0.157653000000
H	-3.940630000000	2.902406000000	2.281386000000	C	-2.264748000000	4.020581000000	-1.240931000000
C	-5.452039000000	2.143822000000	0.153191000000	H	-1.786698000000	4.073597000000	-2.214505000000
H	-6.093962000000	2.437068000000	-0.684154000000	C	-3.446186000000	3.278135000000	-1.136475000000
H	-6.010113000000	2.340919000000	1.075323000000	C	-4.116528000000	3.205630000000	0.098216000000
C	-5.167425000000	0.664897000000	0.060241000000	C	-3.548879000000	3.868136000000	1.193598000000
C	-4.978051000000	0.051764000000	-1.250376000000	H	-4.062300000000	3.834238000000	2.154279000000
C	-4.777795000000	-1.378223000000	-1.305458000000	C	-5.436211000000	2.471240000000	0.262721000000
H	-4.676189000000	-1.809627000000	-2.296405000000	H	-6.123348000000	2.751090000000	-0.543623000000
C	-4.714104000000	-2.168592000000	-0.183954000000	H	-5.906839000000	2.811713000000	1.191743000000
C	-4.841373000000	-1.515950000000	1.073302000000	C	-5.309597000000	0.958709000000	0.312884000000
C	-5.080638000000	-0.135769000000	1.181010000000	C	-5.577758000000	0.165066000000	-0.804580000000
H	-5.215161000000	0.300323000000	2.170218000000	C	-5.479183000000	-1.223052000000	-0.744748000000
C	-4.500417000000	-3.667199000000	-0.269683000000	H	-5.702224000000	-1.817251000000	-1.628941000000
H	-4.879639000000	-4.003041000000	-1.240336000000	C	-5.081743000000	-1.872941000000	0.422821000000
H	-5.104206000000	-4.172995000000	0.491315000000	C	-4.789165000000	-1.077621000000	1.539249000000
C	-3.047917000000	-4.098178000000	-0.140965000000	C	-4.910391000000	0.307787000000	1.484749000000
C	-2.206988000000	-4.033768000000	-1.255332000000	H	-4.688959000000	0.905206000000	2.367918000000
H	-2.577154000000	-3.635537000000	-2.196134000000	C	-4.908062000000	-3.375053000000	0.459244000000
C	-0.896000000000	-4.512364000000	-1.225029000000	H	-5.522779000000	-3.817135000000	-0.332897000000
C	-0.396679000000	-5.085499000000	-0.036596000000	H	-5.282954000000	-3.776958000000	1.405794000000
C	-1.224093000000	-5.102483000000	1.087117000000	C	-3.464665000000	-3.804965000000	0.253938000000
H	-0.864389000000	-5.525404000000	2.020952000000	C	-2.903478000000	-3.758817000000	-1.023021000000
C	-2.530569000000	-4.612403000000	1.059133000000	H	-3.475847000000	-3.365790000000	-1.858631000000
C	0.986223000000	-5.709752000000	0.038491000000	C	-1.610198000000	-4.214398000000	-1.277048000000
H	1.128953000000	-6.396321000000	-0.804034000000	C	-0.863709000000	-4.794852000000	-0.233906000000
H	1.031605000000	-6.326603000000	0.942073000000	C	-1.399848000000	-4.773297000000	1.056228000000
H	-3.896221000000	-3.986197000000	2.258839000000	H	-0.832713000000	-5.179578000000	1.889417000000
H	-4.627350000000	2.394499000000	-2.305160000000				
H	-2.168534000000	3.943416000000	3.288052000000				
H	-4.774465000000	-1.753879000000	2.988188000000				



H	0.716359000000	-4.764398000000	-2.304049000000	C	-2.670029000000	-4.260054000000	1.319905000000
C	-1.175343000000	0.985236000000	-2.061296000000	C	0.463605000000	-5.489037000000	-0.493871000000
H	-0.859530000000	0.699198000000	-3.071579000000	H	0.470549000000	-5.877841000000	-1.518073000000
H	-0.579545000000	1.854450000000	-1.755211000000	H	0.522466000000	-6.361509000000	0.165856000000
H	-2.220203000000	1.309133000000	-2.124491000000	H	-5.955811000000	0.182285000000	-2.706319000000
C	-1.006126000000	-0.175074000000	-1.074722000000	H	-3.653962000000	-3.485262000000	2.768575000000
H	0.026183000000	-0.552021000000	-1.113268000000	H	-4.675185000000	2.133495000000	-2.141964000000
H	-1.643197000000	-1.018986000000	-1.375644000000	H	-2.334478000000	5.089658000000	2.953191000000
C	-1.339274000000	0.215096000000	0.370487000000	H	-4.096819000000	-1.083417000000	3.349503000000
H	-2.357010000000	0.625303000000	0.407444000000	H	-0.183005000000	-4.087977000000	-2.574084000000
H	-0.676592000000	1.034681000000	0.683906000000	C	1.848350000000	0.203296000000	-0.794265000000
C	-1.217954000000	-0.960534000000	1.345867000000	H	2.641872000000	-0.492162000000	-0.500700000000
H	-0.203668000000	-1.378416000000	1.342435000000	H	1.765209000000	0.966417000000	-0.011260000000
H	-1.449475000000	-0.658617000000	2.375965000000	H	2.171473000000	0.726094000000	-1.703115000000
H	-1.897542000000	-1.774758000000	1.069841000000	C	0.514295000000	-0.521745000000	-1.001931000000
				H	0.223502000000	-1.036966000000	-0.074962000000
				H	0.630696000000	-1.320581000000	-1.750943000000
				C	-0.616081000000	0.417953000000	-1.441162000000
				H	-0.333687000000	0.897385000000	-2.389910000000
				H	-0.713082000000	1.237509000000	-0.714979000000
				C	-1.965683000000	-0.289370000000	-1.601980000000
				H	-2.318761000000	-0.695575000000	-0.646676000000
				H	-2.726450000000	0.403754000000	-1.977192000000
				H	-1.888127000000	-1.133866000000	-2.298498000000
<b>PA[6]+2-n-butane</b>				<b>PA[6]+1-ethane</b>			
O	-0.894226000000	4.774096000000	-2.336867000000	O	0.209253000000	4.171703000000	-2.454662000000
O	-3.269486000000	3.650395000000	2.535011000000	O	-2.516473000000	5.207543000000	2.262652000000
O	-5.509247000000	-0.870713000000	-2.457450000000	O	-6.160980000000	0.114555000000	-1.915637000000
O	-5.283965000000	1.734519000000	2.424086000000	O	-3.845916000000	2.725808000000	2.384144000000
O	-3.955158000000	-3.223938000000	-2.456100000000	O	-4.984737000000	-2.426825000000	-2.195052000000
O	-2.054820000000	-4.295574000000	2.640281000000	O	-2.495797000000	-4.352353000000	2.371759000000
C	-1.529138000000	4.467068000000	-1.139712000000	C	-0.499432000000	4.427359000000	-1.281206000000

C	-0.814851000000	4.696591000000	0.044336000000	C	0.173593000000	5.050359000000	-0.221692000000
C	-1.448207000000	4.376766000000	1.243119000000	C	-0.547698000000	5.284399000000	0.948964000000
H	-0.932594000000	4.528681000000	2.186822000000	H	-0.061065000000	5.737750000000	1.807582000000
C	-2.759835000000	3.890284000000	1.292752000000	C	-1.897826000000	4.943174000000	1.068532000000
C	-3.495136000000	3.740561000000	0.103662000000	C	-2.585039000000	4.403692000000	-0.031635000000
C	-2.844234000000	4.016194000000	-1.106288000000	C	-1.855028000000	4.129671000000	-1.193262000000
H	-3.394051000000	3.902050000000	-2.040159000000	H	-2.363481000000	3.702843000000	-2.056028000000
C	-4.965625000000	3.343561000000	0.103896000000	C	-4.091653000000	4.201395000000	-0.007296000000
H	-5.457006000000	3.765932000000	0.987022000000	H	-4.515295000000	4.791139000000	0.813246000000
H	-5.446826000000	3.808209000000	-0.763966000000	H	-4.511613000000	4.618461000000	-0.929885000000
C	-5.219754000000	1.846797000000	0.046471000000	C	-4.544329000000	2.761578000000	0.112953000000
C	-5.345924000000	1.074018000000	1.205703000000	C	-4.396565000000	2.049203000000	1.310107000000
C	-5.530256000000	-0.304324000000	1.140725000000	C	-4.818633000000	0.727008000000	1.416732000000
H	-5.612060000000	-0.878231000000	2.061740000000	H	-4.694203000000	0.194888000000	2.358388000000
C	-5.574801000000	-0.978621000000	-0.080897000000	C	-5.408176000000	0.057945000000	0.339485000000
C	-5.457287000000	-0.205939000000	-1.241587000000	C	-5.556451000000	0.770592000000	-0.854256000000
C	-5.296010000000	1.175926000000	-1.176637000000	C	-5.132929000000	2.094538000000	-0.962388000000
H	-5.202838000000	1.747535000000	-2.098485000000	H	-5.272777000000	2.628566000000	-1.901171000000
C	-5.656040000000	-2.494499000000	-0.126517000000	C	-5.854990000000	-1.388095000000	0.468817000000
H	-6.269297000000	-2.837074000000	0.713985000000	H	-6.261521000000	-1.535542000000	1.475225000000
H	-6.170613000000	-2.816629000000	-1.037509000000	H	-6.680113000000	-1.578377000000	-0.226206000000
C	-4.288421000000	-3.155955000000	-0.031606000000	C	-4.743194000000	-2.402137000000	0.247392000000
C	-3.737146000000	-3.434826000000	1.222021000000	C	-4.058557000000	-2.930709000000	1.345425000000
H	-4.282705000000	-3.182969000000	2.127724000000	H	-4.314565000000	-2.609112000000	2.351791000000
C	-2.490973000000	-4.045720000000	1.365845000000	C	-3.063543000000	-3.901137000000	1.211961000000
C	-1.777166000000	-4.444789000000	0.219461000000	C	-2.739595000000	-4.381539000000	-0.071624000000
C	-2.301751000000	-4.114564000000	-1.031678000000	C	-3.402583000000	-3.830500000000	-1.169867000000
H	-1.767243000000	-4.390493000000	-1.936641000000	H	-3.174618000000	-4.180842000000	-2.172846000000
C	-3.530379000000	-3.466493000000	-1.175410000000	C	-4.386398000000	-2.848405000000	-1.038075000000
C	-0.540778000000	-5.325939000000	0.319787000000	C	-1.730648000000	-5.497010000000	-0.286287000000
H	-0.582996000000	-5.875708000000	1.267456000000	H	-1.912305000000	-6.305512000000	0.431223000000
H	-0.608696000000	-6.080848000000	-0.470946000000	H	-1.905726000000	-5.927007000000	-1.278070000000

H	-5.182855000000	1.085926000000	3.138202000000	H	-3.666394000000	2.105789000000	3.106828000000
H	-4.594992000000	-2.487773000000	-2.466486000000	H	-5.471105000000	-1.592676000000	-2.058974000000
H	-4.039785000000	3.050779000000	2.487442000000	H	-3.137580000000	4.475968000000	2.440165000000
H	-1.437594000000	4.473056000000	-3.080242000000	H	-0.098102000000	3.332188000000	-2.830399000000
H	-5.198261000000	-0.280588000000	-3.161218000000	H	-6.114374000000	0.668025000000	-2.710156000000
H	-1.078004000000	-4.272465000000	2.648081000000	H	-1.750484000000	-4.958764000000	2.200613000000
O	0.731362000000	-3.987267000000	2.487104000000	O	-0.153884000000	-5.897015000000	2.027662000000
O	3.460677000000	-4.316075000000	-2.321177000000	O	2.222998000000	-3.581279000000	-2.408268000000
O	6.038807000000	0.938119000000	2.272375000000	O	4.780537000000	-0.170715000000	2.722586000000
O	4.693906000000	-1.804551000000	-2.349473000000	O	4.874067000000	-2.614200000000	-2.246977000000
O	4.103680000000	3.019329000000	2.413476000000	O	4.169813000000	2.607130000000	2.738081000000
O	1.903985000000	4.475831000000	-2.462612000000	O	2.985743000000	3.974432000000	-2.505053000000
C	1.451266000000	-4.071164000000	1.302135000000	C	0.491501000000	-5.311843000000	0.943035000000
C	0.823881000000	-4.669271000000	0.200046000000	C	-0.271524000000	-5.077775000000	-0.206656000000
C	1.540000000000	-4.711341000000	-0.995678000000	C	0.364715000000	-4.474286000000	-1.290262000000
H	1.088560000000	-5.142329000000	-1.884673000000	H	-0.195316000000	-4.263670000000	-2.196663000000
C	2.849132000000	-4.227305000000	-1.100138000000	C	1.723812000000	-4.142652000000	-1.269279000000
C	3.505300000000	-3.737883000000	0.041266000000	C	2.493881000000	-4.430209000000	-0.126241000000
C	2.772314000000	-3.644258000000	1.230127000000	C	1.846807000000	-5.002452000000	0.975304000000
H	3.255107000000	-3.247543000000	2.121626000000	H	2.428378000000	-5.237076000000	1.866431000000
C	4.977718000000	-3.355261000000	0.018536000000	C	3.993854000000	-4.194405000000	-0.078191000000
H	5.461893000000	-3.841615000000	-0.834643000000	H	4.462667000000	-4.608749000000	-0.977863000000
H	5.456921000000	-3.762703000000	0.916193000000	H	4.403134000000	-4.765500000000	0.762618000000
C	5.231661000000	-1.860920000000	-0.022016000000	C	4.419561000000	-2.745125000000	0.080832000000
C	5.062501000000	-1.121841000000	-1.198845000000	C	4.881857000000	-1.996166000000	-1.004919000000
C	5.257512000000	0.255497000000	-1.218176000000	C	5.335872000000	-0.690100000000	-0.840046000000
H	5.125679000000	0.801360000000	-2.149293000000	H	5.704574000000	-0.135570000000	-1.700893000000
C	5.577096000000	0.965040000000	-0.058000000000	C	5.312151000000	-0.063933000000	0.406784000000
C	5.735502000000	0.229566000000	1.120403000000	C	4.808332000000	-0.798726000000	1.488082000000
C	5.588588000000	-1.157446000000	1.130795000000	C	4.384079000000	-2.115245000000	1.328035000000
H	5.729141000000	-1.704834000000	2.061747000000	H	4.017200000000	-2.673389000000	2.188083000000
C	5.660590000000	2.481406000000	-0.077673000000	C	5.757622000000	1.376510000000	0.560946000000

H	6.165766000000	2.793646000000	-0.998026000000	H	6.543711000000	1.577937000000	-0.175143000000
H	6.284325000000	2.831545000000	0.751294000000	H	6.208104000000	1.526543000000	1.547094000000
C	4.292409000000	3.144781000000	-0.029648000000	C	4.627489000000	2.371013000000	0.349712000000
C	3.655238000000	3.507598000000	-1.219475000000	C	4.266658000000	2.742517000000	-0.947043000000
H	4.139759000000	3.324609000000	-2.175045000000	H	4.772120000000	2.303660000000	-1.803152000000
C	2.409087000000	4.137681000000	-1.237139000000	C	3.267072000000	3.681921000000	-1.195171000000
C	1.783460000000	4.464072000000	-0.018604000000	C	2.625894000000	4.314703000000	-0.114466000000
C	2.392200000000	4.046029000000	1.167326000000	C	2.947416000000	3.901787000000	1.180506000000
H	1.927170000000	4.267576000000	2.124205000000	H	2.445246000000	4.347825000000	2.034725000000
C	3.616556000000	3.374108000000	1.183158000000	C	3.916247000000	2.927698000000	1.428116000000
C	0.553379000000	5.358807000000	0.033702000000	C	1.634065000000	5.446559000000	-0.329364000000
H	0.596015000000	6.061950000000	-0.806271000000	H	1.819997000000	5.908814000000	-1.305039000000
H	0.627181000000	5.966881000000	0.941555000000	H	1.830304000000	6.221847000000	0.419198000000
H	4.155556000000	-1.219114000000	-2.905900000000	H	5.085440000000	-1.962281000000	-2.933283000000
H	4.840888000000	2.385873000000	2.335061000000	H	4.457045000000	1.676444000000	2.792405000000
H	4.046780000000	-3.540212000000	-2.421843000000	H	3.167026000000	-3.346011000000	-2.325743000000
H	1.160100000000	-3.352226000000	3.080160000000	H	0.445777000000	-5.912905000000	2.788845000000
H	5.996547000000	0.344641000000	3.037908000000	H	4.295740000000	-0.720687000000	3.356549000000
H	0.937995000000	4.611068000000	-2.407848000000	H	2.035322000000	4.198220000000	-2.570321000000
C	-1.891265000000	-0.276450000000	-2.057046000000	C	0.993106000000	1.068048000000	-1.675639000000
H	-1.817115000000	0.396961000000	-2.921466000000	H	1.701654000000	1.566031000000	-2.346960000000
H	-2.842883000000	-0.812953000000	-2.123923000000	H	0.756318000000	1.777667000000	-0.875086000000
H	-1.101574000000	-1.029321000000	-2.156301000000	H	0.067811000000	0.865961000000	-2.233619000000
C	-1.769632000000	0.493323000000	-0.738691000000	C	1.581845000000	-0.225921000000	-1.104375000000
H	-2.565162000000	1.242584000000	-0.677683000000	H	2.501705000000	-0.016695000000	-0.548158000000
H	-0.828927000000	1.057664000000	-0.727179000000	H	0.878997000000	-0.714348000000	-0.419741000000
C	-1.844664000000	-0.410846000000	0.495922000000	H	1.819534000000	-0.951934000000	-1.890366000000
H	-1.049237000000	-1.165854000000	0.451706000000				
H	-2.781792000000	-0.973977000000	0.468575000000				
C	-1.747708000000	0.357300000000	1.816983000000				
H	-2.574934000000	1.065823000000	1.934318000000				
H	-1.769165000000	-0.329417000000	2.672692000000				

H	-0.820855000000	0.939216000000	1.876207000000				
C	1.948161000000	-0.132734000000	1.693815000000				
H	2.060862000000	0.674951000000	2.426594000000				
H	2.816239000000	-0.795469000000	1.785066000000				
H	1.052487000000	-0.712180000000	1.952598000000				
C	1.858067000000	0.431994000000	0.273560000000				
H	2.767861000000	0.999327000000	0.061591000000				
H	1.039578000000	1.159876000000	0.217889000000				
C	1.681948000000	-0.639382000000	-0.806569000000				
H	0.739955000000	-1.179141000000	-0.657070000000				
H	2.468508000000	-1.391879000000	-0.698445000000				
C	1.723975000000	-0.060151000000	-2.223637000000				
H	2.659101000000	0.491378000000	-2.392734000000				
H	1.631013000000	-0.847144000000	-2.983551000000				
H	0.911589000000	0.655948000000	-2.390462000000				
<b>PA[6]+2-ethane</b>				<b>PA[6]+1-propane</b>			
O	-6.097357000000	-0.941114000000	-1.727565000000	O	-2.219436000000	4.763169000000	-2.480514000000
O	-3.171517000000	-3.041037000000	2.480120000000	O	-4.125867000000	2.996607000000	2.410752000000
O	0.927084000000	-4.170472000000	-2.358695000000	O	-4.617769000000	-2.219058000000	-2.392207000000
O	-1.870087000000	-5.553105000000	2.220310000000	O	-5.402727000000	0.508558000000	2.363303000000
O	3.702437000000	-3.683018000000	-2.367774000000	O	-2.993787000000	-4.529816000000	-2.444637000000
O	4.400705000000	-1.974437000000	2.863158000000	O	-0.312973000000	-4.494734000000	2.409740000000
C	-5.339328000000	-1.504747000000	-0.705502000000	C	-2.724952000000	4.280457000000	-1.277889000000
C	-5.201503000000	-0.768378000000	0.475923000000	C	-2.146561000000	4.762619000000	-0.097071000000
C	-4.448972000000	-1.335437000000	1.503722000000	C	-2.646903000000	4.276318000000	1.108695000000
H	-4.319649000000	-0.798925000000	2.439099000000	H	-2.219682000000	4.613255000000	2.048568000000
C	-3.854666000000	-2.596642000000	1.387949000000	C	-3.705273000000	3.362768000000	1.166130000000
C	-3.999779000000	-3.327588000000	0.192959000000	C	-4.316580000000	2.929567000000	-0.024620000000
C	-4.750996000000	-2.756785000000	-0.840150000000	C	-3.792335000000	3.390371000000	-1.238682000000
H	-4.882288000000	-3.313880000000	-1.767164000000	H	-4.255931000000	3.068707000000	-2.171074000000
C	-3.402365000000	-4.710836000000	0.011711000000	C	-5.548343000000	2.038108000000	-0.019927000000
H	-3.765021000000	-5.382248000000	0.798621000000	H	-6.177629000000	2.291744000000	0.840035000000

H	-3.777692000000	-5.125420000000	-0.930524000000	H	-6.143099000000	2.267912000000	-0.911172000000
C	-1.883687000000	-4.763560000000	-0.019062000000	C	-5.261096000000	0.547211000000	-0.011701000000
C	-1.153297000000	-5.234160000000	1.075946000000	C	-5.193150000000	-0.182079000000	1.178959000000
C	0.229850000000	-5.388354000000	1.009692000000	C	-4.955899000000	-1.554731000000	1.172025000000
H	0.768144000000	-5.789720000000	1.866607000000	H	-4.925841000000	-2.099629000000	2.113940000000
C	0.946142000000	-5.042624000000	-0.137175000000	C	-4.751825000000	-2.254875000000	-0.017299000000
C	0.222339000000	-4.509744000000	-1.212852000000	C	-4.798365000000	-1.521999000000	-1.209682000000
C	-1.164516000000	-4.388442000000	-1.157954000000	C	-5.057546000000	-0.153704000000	-1.204116000000
H	-1.704938000000	-4.011539000000	-2.023868000000	H	-5.109702000000	0.387603000000	-2.147598000000
C	2.447804000000	-5.238994000000	-0.202916000000	C	-4.472406000000	-3.744087000000	-0.008224000000
H	2.729519000000	-5.970892000000	0.562448000000	H	-4.913967000000	-4.170516000000	0.899353000000
H	2.718436000000	-5.684122000000	-1.166290000000	H	-4.980597000000	-4.220535000000	-0.853254000000
C	3.263989000000	-3.975602000000	0.015022000000	C	-2.995510000000	-4.106317000000	-0.038961000000
C	3.457082000000	-3.478741000000	1.306148000000	C	-2.250896000000	-4.102602000000	1.142578000000
H	2.979066000000	-3.960909000000	2.154860000000	H	-2.708516000000	-3.782371000000	2.074892000000
C	4.265151000000	-2.368785000000	1.558140000000	C	-0.925190000000	-4.537040000000	1.187217000000
C	4.943902000000	-1.750045000000	0.490978000000	C	-0.318285000000	-5.027227000000	0.014440000000
C	4.708570000000	-2.215915000000	-0.803971000000	C	-1.046110000000	-4.973228000000	-1.176561000000
H	5.190978000000	-1.738379000000	-1.652341000000	H	-0.600470000000	-5.325903000000	-2.102633000000
C	3.868192000000	-3.299108000000	-1.057840000000	C	-2.359269000000	-4.502487000000	-1.227882000000
C	5.903511000000	-0.591898000000	0.712815000000	C	1.072522000000	-5.640443000000	0.019311000000
H	6.342158000000	-0.658351000000	1.713717000000	H	1.189842000000	-6.284080000000	0.898430000000
H	6.731093000000	-0.685340000000	0.001602000000	H	1.155470000000	-6.297851000000	-0.852567000000
H	-1.253227000000	-5.756618000000	2.940513000000	H	-5.181357000000	-0.062561000000	3.115003000000
H	2.782423000000	-3.991985000000	-2.476430000000	H	-3.627075000000	-3.788910000000	-2.485488000000
H	-2.863349000000	-3.961261000000	2.380431000000	H	-4.626558000000	2.157984000000	2.380928000000
H	-6.007356000000	-1.480151000000	-2.528169000000	H	-2.625933000000	4.283283000000	-3.217561000000
H	0.471065000000	-3.450008000000	-2.820725000000	H	-4.540590000000	-1.596431000000	-3.130704000000
H	4.574755000000	-1.013655000000	2.898697000000	H	0.641933000000	-4.689736000000	2.343410000000
O	4.664563000000	0.837600000000	2.825048000000	O	2.483151000000	-4.815911000000	2.330686000000
O	4.564052000000	3.064945000000	-2.247915000000	O	3.983251000000	-2.695369000000	-2.561396000000
O	-0.890348000000	5.992369000000	1.991844000000	O	4.638722000000	2.186886000000	2.422343000000

O	1.892407000000	3.819485000000	-2.276951000000	O	5.398768000000	-0.267933000000	-2.484385000000
O	-3.012982000000	4.135803000000	2.418222000000	O	2.830625000000	4.356205000000	2.519456000000
O	-5.108214000000	1.643220000000	-2.069913000000	O	0.584822000000	5.019105000000	-2.509624000000
C	4.626637000000	1.438813000000	1.572524000000	C	2.905782000000	-4.262933000000	1.125788000000
C	5.253669000000	0.764529000000	0.515844000000	C	2.215929000000	-4.642284000000	-0.030994000000
C	5.203731000000	1.354803000000	-0.745127000000	C	2.613098000000	-4.067966000000	-1.236720000000
H	5.649110000000	0.852877000000	-1.598775000000	H	2.091239000000	-4.320960000000	-2.154899000000
C	4.569168000000	2.579748000000	-0.967440000000	C	3.675478000000	-3.160926000000	-1.317598000000
C	4.001893000000	3.279535000000	0.110520000000	C	4.396015000000	-2.828215000000	-0.154885000000
C	4.024933000000	2.676711000000	1.374210000000	C	3.980894000000	-3.384793000000	1.060284000000
H	3.577985000000	3.200354000000	2.218868000000	H	4.526366000000	-3.136320000000	1.970160000000
C	3.438138000000	4.680327000000	-0.057124000000	C	5.609937000000	-1.915979000000	-0.191790000000
H	3.852365000000	5.121187000000	-0.970724000000	H	6.194938000000	-2.115629000000	-1.096056000000
H	3.800336000000	5.301581000000	0.770116000000	H	6.259108000000	-2.171036000000	0.653264000000
C	1.925110000000	4.774419000000	-0.091138000000	C	5.289106000000	-0.433164000000	-0.115233000000
C	1.188919000000	4.337187000000	-1.199345000000	C	5.200501000000	0.360112000000	-1.263020000000
C	-0.194972000000	4.482563000000	-1.248590000000	C	4.955780000000	1.729211000000	-1.177262000000
H	-0.735522000000	4.168115000000	-2.138822000000	H	4.916424000000	2.326639000000	-2.086430000000
C	-0.906855000000	5.052300000000	-0.189064000000	C	4.767025000000	2.361659000000	0.052956000000
C	-0.176384000000	5.447611000000	0.936174000000	C	4.817873000000	1.559833000000	1.200466000000
C	1.211900000000	5.322891000000	0.976961000000	C	5.081424000000	0.195099000000	1.115454000000
H	1.756637000000	5.672267000000	1.852922000000	H	5.139369000000	-0.399530000000	2.025778000000
C	-2.408298000000	5.265840000000	-0.279992000000	C	4.514738000000	3.855951000000	0.132312000000
H	-2.639805000000	5.631500000000	-1.286205000000	H	5.028293000000	4.334076000000	-0.709159000000
H	-2.700168000000	6.067156000000	0.407901000000	H	4.973570000000	4.256467000000	1.042422000000
C	-3.244012000000	4.025074000000	-0.022073000000	C	3.047128000000	4.251427000000	0.085853000000
C	-3.803608000000	3.333471000000	-1.098545000000	C	2.410010000000	4.418149000000	-1.146147000000
H	-3.626442000000	3.673945000000	-2.115350000000	H	2.949438000000	4.225943000000	-2.070139000000
C	-4.620568000000	2.215633000000	-0.926009000000	C	1.089979000000	4.860317000000	-1.247027000000
C	-4.912780000000	1.769641000000	0.376203000000	C	0.378876000000	5.182024000000	-0.074961000000
C	-4.330974000000	2.446217000000	1.451634000000	C	0.999950000000	4.966243000000	1.156879000000
H	-4.535921000000	2.124654000000	2.469122000000	H	0.469991000000	5.187063000000	2.079440000000

C	-3.497443000000	3.553197000000	1.278840000000	C	2.308734000000	4.492205000000	1.258210000000
C	-5.845973000000	0.598363000000	0.639563000000	C	-1.018296000000	5.779268000000	-0.121789000000
H	-6.724866000000	0.666774000000	-0.011564000000	H	-1.116433000000	6.414288000000	-1.009104000000
H	-6.218500000000	0.681976000000	1.665831000000	H	-1.136807000000	6.438854000000	0.744445000000
H	1.358047000000	3.146672000000	-2.726215000000	H	5.197117000000	0.349940000000	-3.203996000000
H	-2.366756000000	4.837781000000	2.219527000000	H	3.506468000000	3.652854000000	2.519310000000
H	3.702169000000	3.501714000000	-2.395132000000	H	4.535846000000	-1.890687000000	-2.518591000000
H	4.089769000000	1.325412000000	3.433973000000	H	2.937896000000	-4.372829000000	3.063000000000
H	-0.299887000000	6.128530000000	2.748527000000	H	4.562492000000	1.521730000000	3.123085000000
H	-5.543483000000	0.787171000000	-1.890704000000	H	-0.391595000000	4.992229000000	-2.493999000000
C	1.469165000000	-0.943623000000	-2.356121000000	C	-1.544648000000	-0.416400000000	0.654740000000
H	0.830543000000	-0.998896000000	-3.248985000000	H	-1.271192000000	0.552358000000	1.092659000000
H	0.938569000000	-1.427738000000	-1.528170000000	H	-1.905071000000	-1.064709000000	1.462550000000
H	2.376810000000	-1.520602000000	-2.551870000000	H	-2.383918000000	-0.247146000000	-0.028503000000
C	1.797731000000	0.509123000000	-2.004915000000	C	-0.352416000000	-1.060382000000	-0.059465000000
H	0.881297000000	1.085075000000	-1.823587000000	H	-0.666967000000	-2.009567000000	-0.512230000000
H	2.405162000000	0.566171000000	-1.096683000000	H	-0.027614000000	-0.411424000000	-0.885018000000
H	2.375014000000	0.993195000000	-2.802283000000	C	0.831840000000	-1.319729000000	0.877566000000
C	-1.507499000000	0.481425000000	-0.273232000000	H	0.553757000000	-2.030990000000	1.665325000000
H	-0.554384000000	0.065174000000	0.074821000000	H	1.685507000000	-1.737666000000	0.334651000000
H	-2.221800000000	0.428268000000	0.553813000000	H	1.162649000000	-0.389551000000	1.359254000000
H	-1.352216000000	1.542851000000	-0.497925000000				
C	-2.033264000000	-0.277678000000	-1.493802000000				
H	-2.200390000000	-1.334414000000	-1.254257000000				
H	-2.983715000000	0.141068000000	-1.839699000000				
H	-1.324750000000	-0.228734000000	-2.329920000000				
<b>PA[6]+2-propane</b>							
O	4.274138000000	-3.367810000000	-2.102940000000				
O	4.559942000000	-1.114711000000	2.951217000000				
O	3.514303000000	3.713211000000	-2.085066000000				
O	4.737811000000	1.711854000000	2.934426000000				
O	0.948837000000	4.833718000000	-2.368946000000				



O	-1.754013000000	4.825074000000	2.473438000000
C	4.398612000000	-2.781003000000	-0.847276000000
C	3.851057000000	-3.463568000000	0.243805000000
C	3.935197000000	-2.855170000000	1.495937000000
H	3.502110000000	-3.342593000000	2.364627000000
C	4.544104000000	-1.609150000000	1.679808000000
C	5.142018000000	-0.960465000000	0.583540000000
C	5.051039000000	-1.566241000000	-0.672942000000
H	5.509235000000	-1.078055000000	-1.531391000000
C	5.866107000000	0.365711000000	0.721547000000
H	6.385074000000	0.412177000000	1.684496000000
H	6.643305000000	0.419840000000	-0.048847000000
C	4.959540000000	1.574801000000	0.572242000000
C	4.425020000000	2.229675000000	1.686362000000
C	3.642478000000	3.373282000000	1.542441000000
H	3.265503000000	3.883299000000	2.427254000000
C	3.332455000000	3.891042000000	0.282744000000
C	3.821380000000	3.202888000000	-0.834201000000
C	4.629370000000	2.077082000000	-0.689031000000
H	5.026708000000	1.586549000000	-1.575406000000
C	2.504154000000	5.154736000000	0.142480000000
H	2.716974000000	5.798059000000	1.003263000000
H	2.833057000000	5.709436000000	-0.742799000000
C	1.002069000000	4.931202000000	0.076020000000
C	0.254058000000	4.896470000000	1.255133000000
H	0.749832000000	4.985379000000	2.218422000000
C	-1.138456000000	4.797818000000	1.253180000000
C	-1.824468000000	4.753232000000	0.023400000000
C	-1.071463000000	4.730668000000	-1.152876000000
H	-1.571108000000	4.685119000000	-2.116738000000
C	0.321988000000	4.808366000000	-1.148097000000
C	-3.342763000000	4.790664000000	-0.053886000000

H	-3.731582000000	5.452401000000	0.728390000000
H	-3.622422000000	5.247856000000	-1.008772000000
H	4.235236000000	2.182261000000	3.617261000000
H	1.871882000000	4.528685000000	-2.275473000000
H	4.697013000000	-0.147392000000	2.952427000000
H	4.471090000000	-2.703405000000	-2.781552000000
H	3.645683000000	3.024990000000	-2.756505000000
H	-2.675101000000	4.504716000000	2.412145000000
O	-4.330060000000	3.740905000000	2.387937000000
O	-5.020697000000	0.765136000000	-2.232234000000
O	-2.780718000000	-3.420111000000	2.248605000000
O	-5.933502000000	-1.915327000000	-2.058851000000
O	-1.095665000000	-5.637448000000	2.313915000000
O	1.520177000000	-3.884262000000	-2.251614000000
C	-4.512481000000	2.948466000000	1.259432000000
C	-4.031397000000	3.440369000000	0.040595000000
C	-4.224755000000	2.653002000000	-1.093238000000
H	-3.863952000000	2.995479000000	-2.058573000000
C	-4.887188000000	1.421828000000	-1.045028000000
C	-5.389950000000	0.950083000000	0.182010000000
C	-5.179653000000	1.730599000000	1.324546000000
H	-5.567674000000	1.381489000000	2.280830000000
C	-6.135734000000	-0.366956000000	0.294519000000
H	-6.924631000000	-0.425521000000	-0.463514000000
H	-6.644452000000	-0.398045000000	1.264225000000
C	-5.230953000000	-1.581486000000	0.183387000000
C	-5.153895000000	-2.334251000000	-0.992532000000
C	-4.333582000000	-3.457816000000	-1.083498000000
H	-4.316693000000	-4.037681000000	-2.004837000000
C	-3.531681000000	-3.855573000000	-0.011370000000
C	-3.570528000000	-3.071977000000	1.149933000000
C	-4.414287000000	-1.971464000000	1.247447000000

H	-4.424908000000	-1.404844000000	2.174284000000
C	-2.674612000000	-5.101018000000	-0.100021000000
H	-2.889388000000	-5.599508000000	-1.052065000000
H	-2.978741000000	-5.801762000000	0.686167000000
C	-1.176375000000	-4.878430000000	-0.001609000000
C	-0.456881000000	-4.414445000000	-1.105548000000
H	-0.976965000000	-4.133805000000	-2.017683000000
C	0.937264000000	-4.335359000000	-1.100270000000
C	1.652117000000	-4.755736000000	0.039987000000
C	0.924578000000	-5.154805000000	1.164064000000
H	1.444183000000	-5.459714000000	2.068298000000
C	-0.469744000000	-5.204259000000	1.168918000000
C	3.170867000000	-4.810135000000	0.071394000000
H	3.545509000000	-5.293433000000	-0.838065000000
H	3.469930000000	-5.455725000000	0.903730000000
H	-5.721980000000	-2.446096000000	-2.842616000000
H	-1.898147000000	-5.091315000000	2.431183000000
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H	-1.977040000000	-2.870974000000	2.226193000000
H	2.492396000000	-3.822245000000	-2.173206000000
C	2.601626000000	-0.667024000000	-3.194536000000
H	1.754151000000	-1.359013000000	-3.138590000000
H	3.076573000000	-0.660562000000	-2.207558000000
H	3.313469000000	-1.073697000000	-3.927615000000
C	2.161101000000	0.746710000000	-3.585678000000
H	3.060079000000	1.378724000000	-3.695949000000
H	1.696575000000	0.732583000000	-4.580186000000
C	1.198433000000	1.372096000000	-2.571693000000
H	1.648547000000	1.415047000000	-1.573005000000
H	0.906625000000	2.388011000000	-2.854121000000
H	0.287128000000	0.770428000000	-2.488050000000

C	0.840705000000	-0.949529000000	0.423606000000
H	1.271433000000	0.033704000000	0.652285000000
H	0.999542000000	-1.143773000000	-0.642686000000
H	1.404800000000	-1.705222000000	0.978826000000
C	-0.652662000000	-0.994289000000	0.765211000000
H	-1.034270000000	-1.991866000000	0.506699000000
H	-0.779355000000	-0.864673000000	1.852495000000
C	-1.480350000000	0.067902000000	0.031942000000
H	-1.442374000000	-0.090168000000	-1.052429000000
H	-2.534077000000	0.041505000000	0.328454000000
H	-1.100903000000	1.077607000000	0.230852000000