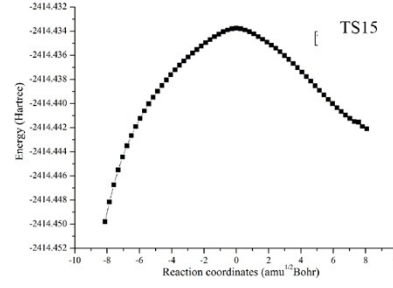
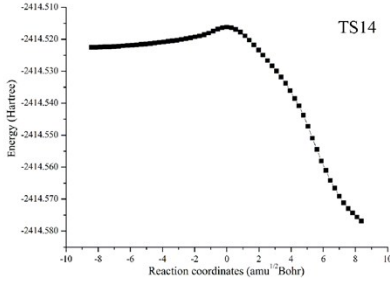
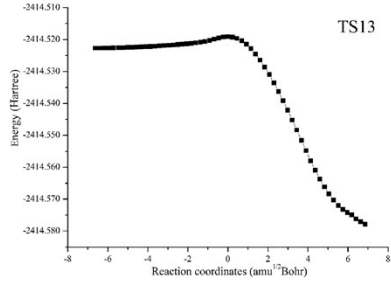
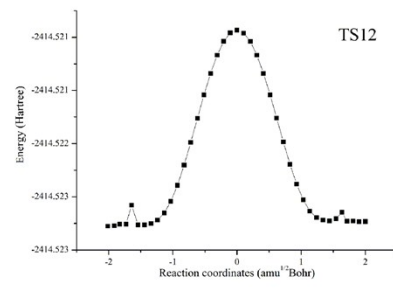
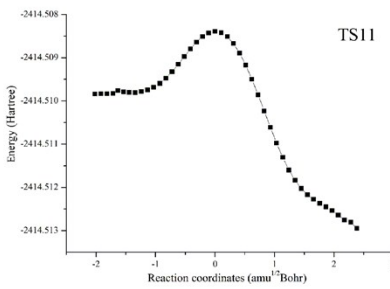
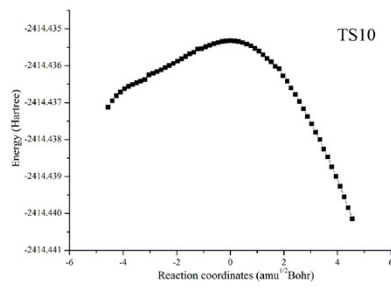
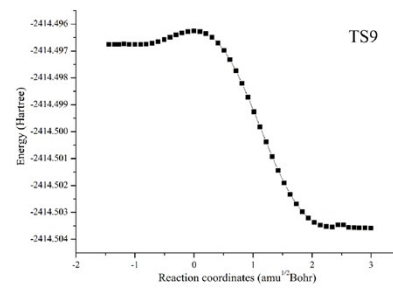
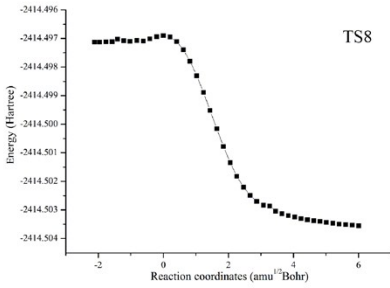
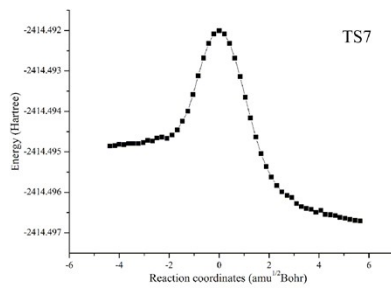
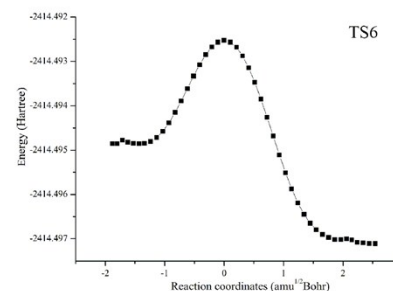
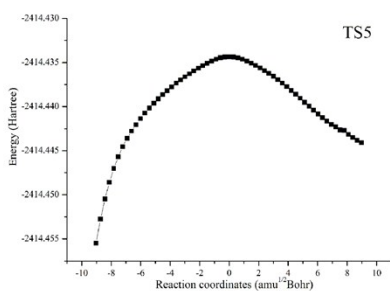
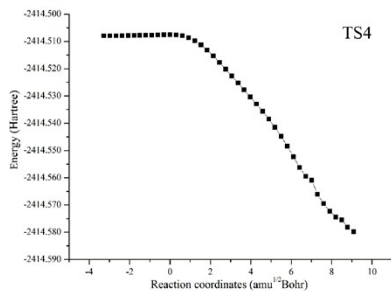
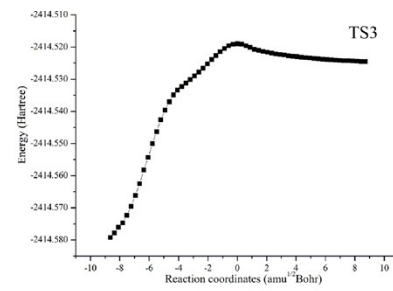
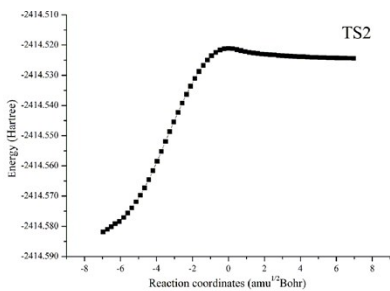
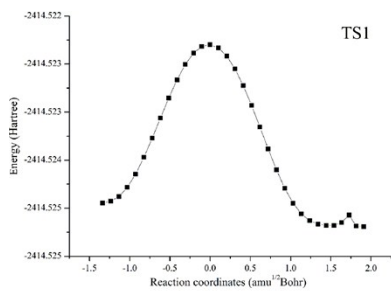


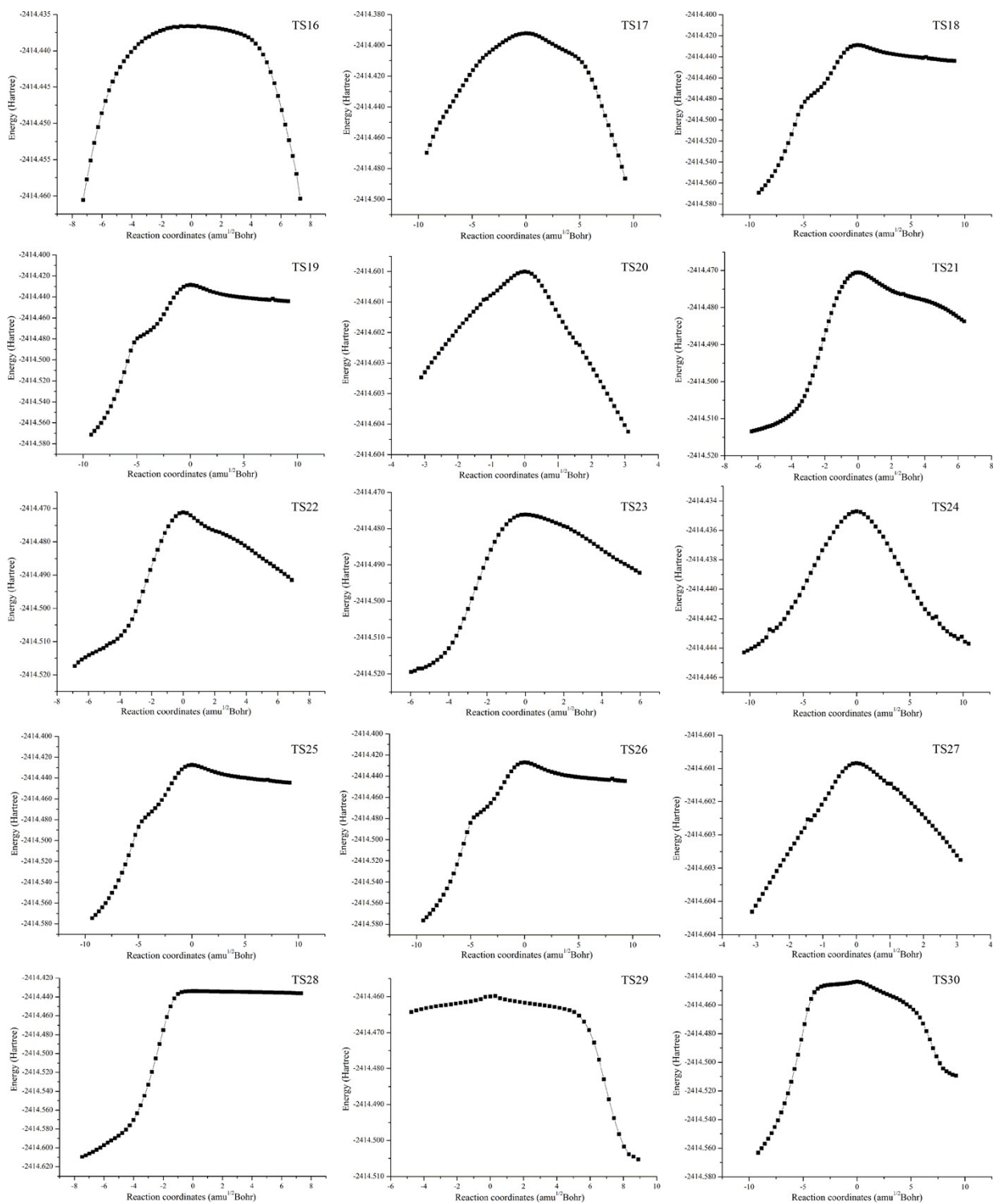
**Theoretical insights into the reaction mechanisms between 2,3,7,8-
tetrachlorodibenzofuran and methylidyne radical**

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Supplementary Material





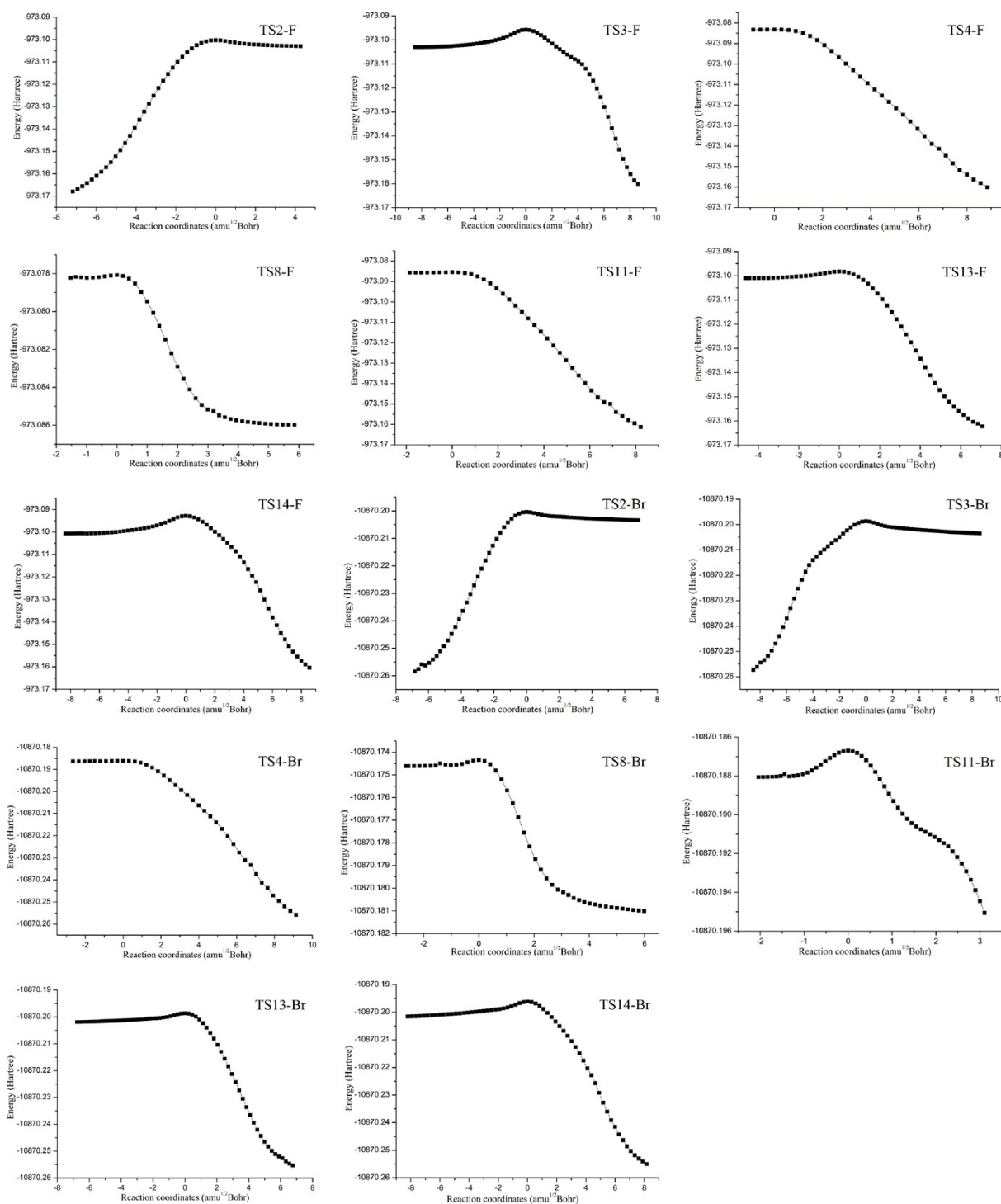


Figure S1. All the IRC calculations on the basis of the corresponding transition states at the B3LYP/6-311++G(d,p) level of theory.

Table S1. The Cartesian coordinates of all the species mentioned in this study

Species	x	y	z	Species	x	y	z
		IM1				IM2	
C	-3.08579800	0.74932800	0.19499300	C	-3.09090500	0.75459400	0.19668600
C	-1.58385800	1.22889400	0.35356000	C	-1.59228700	1.23634300	0.33323400
C	-0.57488600	0.16429400	0.23737700	C	-0.57170800	0.18098100	0.21737600
C	-0.95386400	-1.14451300	0.14899600	C	-0.95586300	-1.12796000	0.13344700
C	-2.29930600	-1.61834400	0.08472100	C	-2.30279400	-1.60296300	0.06588500
C	-3.30719500	-0.71947200	0.07289200	C	-3.31689200	-0.70677200	0.05622900
C	1.22612400	-1.18139000	0.00959200	C	1.22518800	-1.17225700	0.00120700
C	0.85779700	0.17367700	0.12367400	C	0.86120900	0.18451300	0.11125800
C	2.53649800	-1.60784100	-0.09521500	C	2.53439600	-1.60360600	-0.09827000
C	1.86170300	1.14694300	0.12938400	C	1.86852900	1.15431600	0.11913900
C	3.52321500	-0.62384700	-0.09390900	C	3.52454300	-0.62307100	-0.09482400
C	3.18590000	0.74173700	0.01597500	C	3.19169700	0.74400100	0.01169300
O	0.12229500	-1.99032700	0.02557000	O	0.11850700	-1.97730400	0.01486500
H	1.63230400	2.20038300	0.22114100	H	1.64200100	2.20860600	0.20804900
H	-1.33441400	2.17315000	-0.12955300	H	-1.38516400	2.18154900	-0.16558600
H	-2.49851900	-2.68060000	0.03486500	H	-2.49778900	-2.66553600	0.00615400
H	2.79368300	-2.65479200	-0.17910400	H	2.78820900	-2.65155700	-0.17994900
Cl	4.43026900	1.97226900	0.01964400	Cl	4.44048400	1.96974100	0.01800600
Cl	5.18892200	-1.13066100	-0.23236300	Cl	5.18885000	-1.13603000	-0.22601600
Cl	-4.15665300	1.78387300	-0.82715500	Cl	-4.18322800	1.82265700	-0.76839700
Cl	-4.96017700	-1.27237000	-0.01213000	Cl	-4.96556100	-1.26738700	-0.04779300
C	-2.58374900	1.31483900	1.43273100	C	-2.55623100	1.28258200	1.44072100
H	-2.92701900	2.13577900	2.04352300	H	-2.57785700	0.92847700	2.46113000
		IM3				IM4	
C	-3.07161000	0.72453400	-0.09645800	C	-2.87550600	0.85185500	0.03235400
C	-1.76143900	1.29318500	0.27448200	C	-1.64807600	1.21210200	0.45341600
C	-0.62460800	0.19997400	0.64484100	C	-0.69245900	0.20625400	0.93947400
C	-1.04307400	-1.19763200	0.42773400	C	-1.11964100	-1.31188700	0.76671700
C	-2.30980400	-1.60081900	0.22190000	C	-2.41183400	-1.56988700	0.12986200
C	-3.33818100	-0.60342000	0.00413800	C	-3.25999400	-0.55628600	-0.13155600
C	1.15768600	-1.17368800	0.16293300	C	1.05654800	-1.17680200	0.19353700
C	0.82748400	0.17295600	0.32723900	C	0.74680100	0.14891000	0.54038900
C	2.44667000	-1.60358700	-0.08144100	C	2.32466800	-1.54868300	-0.21281400
C	1.82054400	1.13551600	0.26033800	C	1.72752800	1.12490700	0.46140200
C	3.44158200	-0.62528000	-0.16496300	C	3.30723600	-0.55694500	-0.28502700
C	3.13378100	0.73268600	0.00284200	C	3.01406300	0.77222200	0.04499400
O	0.06494700	-2.00725500	0.27468000	O	0.00003700	-2.05089500	0.26186600
H	1.60437800	2.18664900	0.40184700	H	1.52041400	2.15506100	0.72168500
H	-1.44123200	2.17827900	-0.27082600	H	-1.33793200	2.24865100	0.39628600
H	-2.54933300	-2.64262400	0.06055000	H	-2.66496700	-2.59136600	-0.12606000
H	2.68466200	-2.65056600	-0.20918900	H	2.55189600	-2.57148100	-0.48011300

CI	4.37279600	1.96198000	-0.09596000	CI	4.23341000	2.02254400	-0.03842100
CI	5.07618300	-1.14688500	-0.48542700	CI	4.90608000	-1.02658100	-0.80476400
CI	-4.24396700	1.88705300	-0.66457100	CI	-3.99862500	2.10173300	-0.46197600
CI	-4.94067200	-1.23308200	-0.30823400	CI	-4.83723200	-0.93351800	-0.78893000
C	-1.26843000	1.07060600	1.62970300	C	-0.98119200	-0.70565600	2.07860300
H	-1.77543700	0.86199900	2.56171700	H	-0.36032800	-0.96533600	2.92474100
		IM5				IM6	
C	-2.87408200	0.84759900	0.02850600	C	-2.93988400	0.84862000	0.09671200
C	-1.63627400	1.22810700	0.41411800	C	-1.56253300	1.16819000	0.38471500
C	-0.68317200	0.23327300	0.91141000	C	-0.63046000	0.18845600	0.49919900
C	-1.10954200	-1.32527900	0.73953400	C	-1.01574900	-1.23357900	0.56196100
C	-2.38867400	-1.58435000	0.09922600	C	-2.50736800	-1.59052700	0.13793900
C	-3.24976500	-0.56496600	-0.12964900	C	-3.36186600	-0.42277800	-0.14372200
C	1.07487000	-1.17529000	0.19807500	C	1.17071700	-1.16262300	0.11351100
C	0.75662200	0.15196700	0.51213400	C	0.81301400	0.17543900	0.34786600
C	2.35231700	-1.55640400	-0.17172200	C	2.47000700	-1.54445600	-0.16915000
C	1.73403300	1.12956700	0.42676600	C	1.79278200	1.16380300	0.30541900
C	3.33229200	-0.56458100	-0.25184500	C	3.44440300	-0.54508100	-0.19553400
C	3.02803900	0.77124700	0.03886400	C	3.11091000	0.79994200	0.04263800
O	0.01558500	-2.04309800	0.25515500	O	0.11186900	-2.02351700	0.17509400
H	1.52099100	2.16422300	0.66281500	H	1.55264800	2.20524600	0.47562100
H	-1.33475900	2.26418000	0.31851900	H	-1.27885600	2.21249600	0.36461700
H	-2.63651300	-2.59699000	-0.19388200	H	-2.66339300	-2.47297200	-0.47947800
H	2.58618100	-2.58543200	-0.40739700	H	2.72998600	-2.57735000	-0.35491300
CI	4.24322700	2.02490900	-0.05819000	CI	4.33054400	2.05315700	0.01358800
CI	4.94192100	-1.04035100	-0.73429600	CI	5.09104200	-1.01731700	-0.52628800
CI	-4.01724100	2.08475000	-0.45431800	CI	-4.00992700	2.21776200	-0.12266600
CI	-4.83244100	-0.94899200	-0.76875600	CI	-4.92662000	-0.78479100	-0.82068200
C	-1.02899200	-0.65989100	2.03040400	C	-1.97696900	-1.78294900	1.49522600
H	-1.80955600	-0.53258700	2.76829200	H	-2.32302600	-1.52382600	2.48554400
		IM7				IM8	
C	-2.89538400	0.90622300	0.12761700	C	-2.90560600	0.89642600	0.10656600
C	-1.58893600	1.22692000	0.20533100	C	-1.59534200	1.21368700	0.17853200
C	-0.58119000	0.19511500	0.23757200	C	-0.58543300	0.18059900	0.21380800
C	-0.93581900	-1.12164900	0.27221300	C	-0.93393400	-1.13902800	0.23890500
C	-2.30085400	-1.63097800	0.31302800	C	-2.30530100	-1.63700700	0.28395300
C	-3.39703900	-0.49860700	0.14463700	C	-3.39714900	-0.50669000	0.14673800
C	1.24062600	-1.14450600	0.09300600	C	1.24334400	-1.15135000	0.07707100
C	0.86198100	0.20801800	0.13814400	C	0.85815400	0.19961900	0.12182100
C	2.55115700	-1.56991300	-0.00710900	C	2.55618200	-1.57087700	-0.01659600
C	1.85596800	1.18586800	0.07253100	C	1.84850200	1.18180800	0.06327400
C	3.53099600	-0.58085100	-0.06906400	C	3.53214500	-0.57753200	-0.07091900
C	3.18385800	0.78484200	-0.02963200	C	3.17868800	0.78661600	-0.03127100
O	0.13771200	-1.96182400	0.16586000	O	0.14351300	-1.97373400	0.14184800

H	1.61986100	2.24144200	0.10074800	H	1.60782600	2.23635800	0.09130000
H	-1.29855400	2.26941900	0.23774000	H	-1.30169400	2.25560600	0.19917800
H	-2.46582500	-2.57023500	-0.21313600	H	-2.51093300	-2.55871100	-0.25714800
H	2.81417700	-2.61828700	-0.03829200	H	2.82376500	-2.61808000	-0.04857200
Cl	4.41693800	2.02372700	-0.10991400	Cl	4.40682500	2.03092000	-0.10135300
Cl	5.19914700	-1.08376800	-0.19746300	Cl	5.20310000	-1.07290700	-0.19024600
Cl	-4.10766900	2.16799100	0.09584100	Cl	-4.11170200	2.16273800	0.05963600
Cl	-4.75390400	-0.85957200	-0.98957300	Cl	-4.80193000	-0.89252700	-0.92090000
C	-3.29121500	-1.28585700	1.35470500	C	-3.23727700	-1.27571100	1.36649000
H	-4.00297100	-1.89792400	1.88704500	H	-3.14589400	-1.00846800	2.40888600
		IM9				IM10	
C	-2.75806900	1.08500500	0.00005000	C	-2.90633300	0.42801000	-0.00004300
C	-1.40435600	1.40195800	0.00003600	C	-1.61532100	0.92353900	-0.00007600
C	-0.47418000	0.36227300	-0.00000200	C	-0.57163900	-0.00119900	-0.00010200
C	-0.92882900	-0.96752200	0.00000300	C	-0.86750700	-1.37471300	-0.00004300
C	-2.26686500	-1.31663800	0.00002500	C	-2.15709400	-1.87665300	0.00000800
C	-3.16214700	-0.25957800	0.00004100	C	-3.19383800	-0.94613900	-0.00000700
C	1.25887800	-1.10096300	-0.00003500	C	1.32161200	-1.25082800	-0.00001800
C	0.97239200	0.27337100	-0.00009700	C	0.87561300	0.07965100	0.00000400
C	2.54563000	-1.60620700	-0.00000200	C	2.65769400	-1.60272400	-0.00000300
C	2.02602800	1.18632200	-0.00011300	C	1.81398900	1.11037700	0.00001300
C	3.58844200	-0.68138600	-0.00001200	C	3.58486400	-0.56140200	0.00002900
C	3.33069500	0.70461100	-0.00006600	C	3.16646400	0.78443100	0.00002100
O	0.11475900	-1.85938300	-0.00002100	O	0.27075600	-2.13944800	-0.00004200
H	1.85294000	2.25453500	-0.00012700	H	1.51373700	2.15001300	-0.00001800
H	-1.09982300	2.44033400	0.00000200	H	-1.47339300	1.99941300	-0.00007300
H	-2.63591700	-2.33685400	-0.00000900	H	-2.36035400	-2.93859400	0.00004500
H	2.74276900	-2.66929400	0.00004800	H	2.97909000	-2.63500500	-0.00001900
Cl	4.64182300	1.86119900	-0.00001600	Cl	4.33333600	2.08585900	-0.00001200
Cl	5.22335400	-1.28973000	0.00008300	Cl	5.27991100	-0.97541100	0.00003500
Cl	-3.93222600	2.38227900	0.00003200	Cl	-4.26080900	1.58851300	-0.00003500
Cl	-4.90269800	-0.63331200	0.00001800	Cl	-4.84113100	-1.52663200	0.00005900
C	-4.93414500	-2.68025300	-0.00009800	C	-3.31130800	3.40187500	0.00019600
H	-6.05321700	-2.66703600	-0.00011900	H	-4.30051100	3.92481900	-0.00025800
		P1				P2	
C	-3.55993400	0.75383000	0.00015900	C	-2.94471600	0.80285100	0.02597300
C	-1.18307500	1.66617400	0.00002900	C	-1.60261900	1.28475800	0.14992500
C	-0.39211700	0.47072800	-0.00017300	C	-0.65610500	0.55823600	0.82045400
C	-0.89053300	-0.83852000	0.00008000	C	-1.18699700	-1.52018400	0.63073800
C	-2.18560100	-1.36329000	-0.00021600	C	-2.30987300	-1.60796000	-0.13548700
C	-3.38659100	-0.62316900	-0.00020400	C	-3.27019600	-0.54574700	-0.11193300
C	1.30998000	-1.02859600	0.00028000	C	1.04811200	-1.08954200	0.24671900
C	1.03863400	0.34931800	0.00004800	C	0.75605100	0.28850900	0.45283200
C	2.58006700	-1.56274500	0.00040000	C	2.33488400	-1.50790800	-0.05279500

C	2.11479300	1.24428600	-0.00025300	C	1.79315400	1.20944500	0.31971900
C	3.64412700	-0.65625400	0.00016600	C	3.35471300	-0.56682800	-0.17397300
C	3.40842700	0.73301800	-0.00016600	C	3.08457700	0.79540300	0.00499700
O	0.14014800	-1.74448000	0.00031300	O	0.04477200	-2.05424200	0.25450100
H	1.96704800	2.31604700	-0.00052300	H	1.60158200	2.26206500	0.48338100
H	-0.63200500	2.60076800	0.00009900	H	-1.32874600	2.14310200	-0.45528900
H	-2.26592400	-2.44106900	-0.00047900	H	-2.42231000	-2.38982900	-0.87794600
H	2.75599800	-2.62950400	0.00059800	H	2.53690700	-2.55887100	-0.20968700
Cl	4.74277000	1.86473300	-0.00050900	Cl	4.33993700	2.00176900	-0.13684200
Cl	5.26743800	-1.29752900	0.00034700	Cl	4.95913600	-1.13150900	-0.56066300
Cl	-5.18459500	1.42078400	0.00062800	Cl	-4.16049700	2.03362900	-0.28786000
Cl	-4.81263700	-1.64633400	-0.00068300	Cl	-4.89692600	-1.00204900	-0.59553100
C	-2.53701500	1.77499300	0.00007100	C	-1.09144300	-0.53838700	1.69131300
H	-2.93385500	2.78283500	0.00017600	H	-0.71092400	-0.72967100	2.68784700
		P3				P4	
C	-2.91732500	0.80400800	0.05225100	C	-2.89699500	0.76954000	0.00003800
C	-1.59734400	1.31093800	0.20852100	C	-1.53688900	0.87707900	0.00068600
C	-0.63558500	0.54003500	0.83702500	C	-0.55220400	-0.17212300	0.00039600
C	-1.16927200	-1.52330000	0.65027200	C	-0.77775400	-1.54511400	0.00028700
C	-2.33236100	-1.64895000	-0.08128400	C	-3.25228100	-1.75423600	-0.00010200
C	-3.25183300	-0.56585800	-0.09182000	C	-3.70212800	-0.43303900	-0.00012400
C	1.05887400	-1.09186500	0.24959000	C	1.41236800	-1.30852900	0.00019600
C	0.76294100	0.28010200	0.44896800	C	0.87726800	-0.01052100	0.00037500
C	2.34728800	-1.51633500	-0.03529900	C	2.76339000	-1.58434700	-0.00004700
C	1.79354400	1.20543900	0.30360000	C	1.75737800	1.07784000	0.00025000
C	3.36427500	-0.57390100	-0.15943900	C	3.62837600	-0.48825300	-0.00010500
C	3.08719900	0.79021600	0.00034500	C	3.12532100	0.82920400	0.00004300
O	0.03899000	-2.02724300	0.21924100	O	0.40464800	-2.23673800	0.00011500
H	1.60058500	2.25918900	0.45773100	H	1.40327500	2.10017800	0.00038400
H	-1.34903600	2.22277900	-0.32430600	H	-1.14398500	1.88591400	0.00113400
H	-2.49367200	-2.47483700	-0.76417000	H	-4.05077000	-2.48781300	-0.00025900
H	2.55047900	-2.56819100	-0.18428400	H	3.14436700	-2.59610800	-0.00022900
Cl	4.33903600	1.99885100	-0.15263100	Cl	4.21329100	2.19897600	-0.00003200
Cl	4.97351300	-1.13624500	-0.53116200	Cl	5.34605200	-0.79874300	-0.00035100
Cl	-4.13723200	2.01875100	-0.30882900	Cl	-3.75158600	2.30773600	-0.00019300
Cl	-4.87053600	-0.98469300	-0.63414200	Cl	-5.45268000	-0.26256600	-0.00026700
C	-1.14203600	-0.52578700	1.68473200	C	-1.97161400	-2.29249800	0.00014500
H	-2.01175300	-0.37273100	2.31130100	H	-1.87180500	-3.37014800	0.00013900
		P5				P6	
C	-2.79542300	1.43003900	-0.00010900	C	-3.65763700	0.69251300	-0.00005700
C	-1.43290900	1.39521400	0.00028600	C	-2.49456100	1.44367400	-0.00005900
C	-0.61312800	0.21576200	0.00014800	C	-1.22280600	0.83130400	0.00007700
C	-1.03915000	-1.11543500	-0.00026300	C	-1.18930200	-0.58494500	0.00000300
C	-2.31303800	-1.71024700	-0.00022100	C	-2.34554400	-1.34417000	0.00015000

C	-3.50963100	-0.99269500	0.00004200	C	-3.58848800	-0.71055400	0.00012300
C	1.16562300	-1.19571000	-0.00028700	C	1.18929500	-0.58479200	0.00007900
C	0.82417400	0.16528800	0.00012500	C	1.22277700	0.83147000	0.00035600
C	2.46285400	-1.66304400	-0.00044100	C	2.34550400	-1.34410200	0.00001500
C	1.85113300	1.11604700	0.00039900	C	2.49462900	1.44372200	0.00029300
C	3.47674000	-0.70249200	-0.00015300	C	3.58848600	-0.71057600	0.00004600
C	3.16914600	0.67381800	0.00026400	C	3.65767500	0.69254100	0.00013900
O	0.03494100	-1.96872900	-0.00053100	O	0.00002700	-1.26782600	-0.00044500
H	1.64696800	2.17847600	0.00071800	H	2.56215900	2.52419900	0.00043600
H	-0.91349600	2.34500900	0.00053700	H	-2.56195900	2.52415100	-0.00005100
H	-2.35051900	-2.79035000	-0.00009100	H	-2.27965000	-2.42383400	0.00023100
H	2.69450200	-2.71913200	-0.00077300	H	2.27947400	-2.42375500	-0.00011600
Cl	4.44263900	1.87297500	0.00060500	Cl	5.19550300	1.52239200	-0.00001900
Cl	5.13139800	-1.25662900	-0.00032100	Cl	5.02496900	-1.69607500	-0.00019400
Cl	-3.52691500	3.03898400	-0.00064300	Cl	-5.19548200	1.52240000	-0.00032200
Cl	-4.95750800	-2.00153200	0.00067100	Cl	-5.02498000	-1.69601500	0.00022500
C	-3.76036300	0.37392100	-0.00004600	C	-0.00006600	1.54666400	0.00019600
H	-4.79658300	0.67845400	0.00009500	H	-0.00017000	2.62941800	0.00018800
		P7				P8	
C	-2.72368800	0.73595600	-0.00006600	C	-2.69194800	1.23146800	-0.00001500
C	-1.39760100	1.13094300	0.00000200	C	-1.34148700	1.50645700	-0.00001800
C	-0.38651600	0.16532700	-0.00003800	C	-0.43623100	0.43553800	-0.00004700
C	-0.75682900	-1.19371700	-0.00009700	C	-0.94238800	-0.87996500	-0.00003400
C	-2.05721200	-1.61832400	-0.00011100	C	-2.27952800	-1.18375700	-0.00003100
C	-3.11577700	-0.64962800	-0.00011300	C	-3.21822400	-0.11028900	-0.00004100
C	1.43894000	-1.17870200	0.00003900	C	1.24416700	-1.08544200	0.00002400
C	1.05636500	0.17557400	0.00015800	C	0.99961700	0.30039900	0.00000200
C	2.75648100	-1.59157400	-0.00001000	C	2.51333800	-1.62940100	0.00003100
C	2.04680400	1.15871600	0.00013600	C	2.08446400	1.17894600	-0.00002500
C	3.73463300	-0.59577000	0.00002000	C	3.58667800	-0.73755000	0.00002400
C	3.38182800	0.76801700	0.00008000	C	3.37287300	0.65528400	-0.00000700
O	0.35030800	-2.01523100	-0.00004200	O	0.07743800	-1.80685900	-0.00000800
H	1.80018600	2.21229200	0.00021800	H	1.94574600	2.25213600	-0.00006900
H	-1.16304800	2.18744400	0.00004300	H	-1.00083800	2.53371200	0.00000500
H	-2.29492400	-2.67427500	-0.00009100	H	-2.62311000	-2.20847800	0.00002500
H	3.02833100	-2.63806500	-0.00008400	H	2.67756500	-2.69805800	0.00003900
Cl	4.61008800	2.01333500	0.00003800	Cl	4.72114400	1.76948700	-0.00003800
Cl	5.40756900	-1.09180800	-0.00003100	Cl	5.20115000	-1.39955500	0.00004100
Cl	-3.90377100	2.03611900	-0.00019900	Cl	-3.79767000	2.59969300	0.00007300
Cl	-5.94364000	-0.44192100	0.00030800	Cl	-5.30241700	-1.91033700	0.00001100
C	-4.40562300	-1.21392100	-0.00022000	C	-4.60268500	-0.33119700	-0.00009200
H	-4.49803000	-2.29024500	-0.00039300	H	-5.32825400	0.46472800	-0.00003400
		P9				P10	
C	-2.80901000	0.60466300	-0.00005000	C	-2.98359500	0.33528900	-0.00009200

C	-1.44234400	1.02515500	0.00058600	C	-1.64582500	0.81602600	-0.00029400
C	-0.40823200	0.10794500	0.00057800	C	-0.58389600	-0.07509600	0.00004400
C	-0.71403500	-1.26465600	0.00008900	C	-0.84011400	-1.45762800	0.00027700
C	-2.01219800	-1.74163000	-0.00010700	C	-2.12170200	-1.98999200	0.00013300
C	-3.04521300	-0.81230800	-0.00011100	C	-3.17239400	-1.09019900	0.00002000
C	1.47627100	-1.16220800	0.00050000	C	1.34496800	-1.27820000	0.00017600
C	1.04312700	0.17321600	0.00088400	C	0.86393000	0.04034300	0.00004900
C	2.80871600	-1.52666900	0.00003300	C	2.68924600	-1.59583200	0.00018200
C	1.99310400	1.19189000	0.00053500	C	1.77700000	1.09266200	0.00004000
C	3.74799300	-0.49533200	-0.00009800	C	3.59095400	-0.53168700	0.00009700
C	3.34345200	0.85316800	0.00014200	C	3.13831000	0.80173100	0.00000400
O	0.41856700	-2.04143500	0.00012400	O	0.31797000	-2.19378300	0.00028800
H	1.70688000	2.23548500	0.00084800	H	1.45302900	2.12516400	-0.00007200
H	-1.23338200	2.08836500	0.00105300	H	-1.47619000	1.88439100	-0.00061500
H	-2.22547500	-2.80168700	-0.00004000	H	-2.29505300	-3.05729800	0.00010800
H	3.11924100	-2.56232500	-0.00033700	H	3.03630700	-2.61978000	0.00021300
Cl	4.52208900	2.14541000	-0.00008900	Cl	4.27088300	2.13440100	-0.00020100
Cl	5.43905700	-0.92743400	-0.00052800	Cl	5.29650000	-0.90338300	-0.00005900
Cl	-5.46311400	1.62170400	-0.00013300	Cl	-3.94172200	2.92275800	0.00027700
Cl	-4.66209800	-1.48941200	-0.00004600	Cl	-4.79716100	-1.75666000	-0.00031900
C	-3.74152400	1.66921600	-0.00098800	C	-4.09536900	1.20097000	-0.00012400
H	-3.36731200	2.68239700	-0.00093100	H	-5.11543200	0.85650000	0.00013300
		P11				P12	
C	-2.89801300	1.00305800	0.00006100	C	-3.03945300	0.60767000	0.00013600
C	-1.54875600	1.36412700	0.00013000	C	-1.68616500	1.10520400	-0.00014900
C	-0.58991300	0.34488100	0.00010100	C	-0.65734700	0.10413200	-0.00038800
C	-1.00326400	-0.98458200	0.00008600	C	-1.00509300	-1.24845600	-0.00024900
C	-2.35482500	-1.41464700	0.00001400	C	-2.30662800	-1.72083600	-0.00005100
C	-3.30405500	-0.33544000	-0.00001800	C	-3.32295700	-0.75797000	0.00010000
C	1.18762000	-1.06419600	0.00015900	C	1.18151400	-1.22922000	-0.00007800
C	0.85990400	0.29987300	0.00020800	C	0.79117900	0.12424400	-0.00007900
C	2.48692400	-1.53402300	0.00006900	C	2.49661200	-1.65090000	0.00001500
C	1.88660600	1.24245600	0.00010300	C	1.79649100	1.09740700	-0.00002600
C	3.50334200	-0.57947800	0.00000500	C	3.48027900	-0.66389200	0.00006000
C	3.20507100	0.79752500	0.00001600	C	3.12925200	0.69968900	0.00003700
O	0.06034000	-1.85030800	0.00012600	O	0.09774600	-2.06542400	-0.00017300
H	1.68331900	2.30528000	0.00011100	H	1.57560000	2.15425400	0.00010600
H	-1.27374700	2.40987200	0.00022900	H	-2.17708000	3.20948500	0.00019500
H	-1.90289600	-3.51395800	0.00005400	H	-2.53365500	-2.77723900	-0.00005700
H	2.71514400	-2.59090700	0.00002100	H	2.75797900	-2.70008500	0.00004000
Cl	4.48240500	1.99213600	-0.00011300	Cl	4.36085300	1.94190900	0.00009700
Cl	5.15579700	-1.14167000	-0.00010300	Cl	5.15087000	-1.16601100	0.00013000
Cl	-4.07643000	2.29800500	-0.00001400	Cl	-4.35412800	1.75539400	0.00023000
Cl	-5.00026600	-0.73258100	-0.00016100	Cl	-4.96978000	-1.34167100	0.00008600

C	-2.68655000	-2.76963700	-0.00002800	C	-1.39487600	2.46593000	-0.00043800
H	-3.71467800	-3.09746500	-0.00020700	H	-0.37450300	2.81541500	-0.00146700
		P13				TS1	
C	-2.91417500	0.87270400	0.00006700	C	-3.08925900	0.75265200	0.19719000
C	-1.52112100	0.93511000	0.00013600	C	-1.58762200	1.24019900	0.32760600
C	-0.74220000	-0.21656300	0.00038200	C	-0.57014000	0.17674400	0.21755100
C	-1.39075700	-1.49453700	0.00059700	C	-0.95360800	-1.13131900	0.12865600
C	-2.81143100	-1.54284000	0.00027400	C	-2.29913100	-1.60843700	0.06792000
C	-3.55579200	-0.38309500	-0.00009300	C	-3.31347200	-0.71498000	0.06912300
C	1.39844800	-1.45202600	0.00012100	C	1.22760600	-1.17483600	-0.00028800
C	0.72262500	-0.21874400	0.00015000	C	0.86276600	0.18144900	0.11256100
C	2.78587800	-1.53033100	0.00011200	C	2.53721700	-1.60507500	-0.09974200
C	1.51311400	0.93816700	0.00007500	C	1.86962400	1.15183400	0.12283300
C	3.54385400	-0.36633200	0.00002900	C	3.52680000	-0.62399900	-0.09342000
C	2.90037100	0.87839300	-0.00007300	C	3.19307600	0.74260300	0.01568200
O	0.73344100	-2.65011200	0.00023100	O	0.12151100	-1.98027400	0.01029200
H	1.04829300	1.91435200	0.00004000	H	1.64257600	2.20587900	0.21337600
H	-1.06166400	1.91428900	-0.00002900	H	-1.35918800	2.17728400	-0.18247400
H	-3.31753800	-2.49978800	0.00012100	H	-2.49293400	-2.67150700	0.01310200
H	3.26373200	-2.50064900	0.00015800	H	2.79174400	-2.65270800	-0.18333200
Cl	3.80643900	2.37136900	-0.00035400	Cl	4.44122400	1.96928200	0.02562100
Cl	5.28157800	-0.49786900	-0.00019200	Cl	5.19163900	-1.13572100	-0.22425400
Cl	-3.82231500	2.36164000	0.00065800	Cl	-4.18729000	1.79629200	-0.80984000
Cl	-5.29854600	-0.50150400	-0.00101500	Cl	-4.96362900	-1.27691900	-0.00489600
C	-0.63081300	-2.65945300	0.00029800	C	-2.56349300	1.30762600	1.41211100
H	-1.03001900	-3.66183400	0.00075100	H	-2.78950400	1.61659500	2.41757200
		TS2				TS3	
C	-3.20345700	0.72419000	0.28039700	C	-3.27163600	0.70935600	0.31490600
C	-1.49169800	1.29197100	0.52905400	C	-1.50311300	1.31964700	0.56037700
C	-0.55741300	0.20972400	0.39479800	C	-0.54561800	0.26673600	0.43757100
C	-0.94748200	-1.11368200	0.39330700	C	-0.95601500	-1.06115900	0.46029800
C	-2.26421700	-1.58929000	0.23007600	C	-2.26478400	-1.54823600	0.25787500
C	-3.29792100	-0.71438500	0.06544500	C	-3.32773700	-0.70013200	0.04512000
C	1.23207300	-1.15997400	0.16207000	C	1.22482200	-1.12900300	0.20451300
C	0.87212900	0.19904100	0.19280300	C	0.87971100	0.23379900	0.20721900
C	2.53709600	-1.59709100	0.03255600	C	2.52393600	-1.58234100	0.07038700
C	1.87419200	1.16619500	0.08697100	C	1.88956000	1.18793000	0.06822400
C	3.52347000	-0.61955900	-0.08508400	C	3.51850700	-0.61798000	-0.08285300
C	3.19263200	0.75078500	-0.06041900	C	3.20209900	0.75585900	-0.08650400
O	0.13255400	-1.96405800	0.28437900	O	0.12023800	-1.92057800	0.35902600
H	1.65034400	2.22440800	0.11837200	H	1.67555900	2.24855300	0.08038000
H	-1.21090700	2.24844700	0.08737200	H	-1.35343800	2.26683300	0.04855600
H	-2.43202500	-2.65144100	0.11131100	H	-2.39587900	-2.61158200	0.10509600
H	2.78972300	-2.64834500	0.01553800	H	2.76580700	-2.63624600	0.07499000

Cl	4.43460600	1.97502100	-0.20434800	Cl	4.45443800	1.96328000	-0.27302700
Cl	5.18050100	-1.14173700	-0.26296200	Cl	5.16749700	-1.16160700	-0.26916200
Cl	-4.29833900	1.77816400	-0.66031600	Cl	-4.33803200	1.82904200	-0.55378700
Cl	-4.84670300	-1.36176300	-0.44023300	Cl	-4.79610100	-1.37790700	-0.63128300
C	-2.61211100	1.30757600	1.45304000	C	-2.59723500	1.18355400	1.49618000
H	-2.99243000	2.16174800	1.99589000	H	-2.58157900	0.69117700	2.46228500
		TS4				TS5	
C	-3.09547900	0.75131600	-0.07965500	C	-2.95350800	0.54470700	-0.26862000
C	-1.83294700	1.35559400	0.31413700	C	-1.63254800	0.98475300	-0.30441100
C	-0.59211200	0.21071500	0.71469500	C	-0.61205900	0.04815000	-0.14268800
C	-1.03701500	-1.15754100	0.48175000	C	-0.94689400	-1.30251900	0.04090200
C	-2.32185500	-1.55695600	0.32514000	C	-2.24998300	-1.76368800	0.07551800
C	-3.35049300	-0.58274200	0.08516100	C	-3.26117400	-0.81690100	-0.08199200
C	1.15115200	-1.16217300	0.14120700	C	1.24418500	-1.23551200	0.08380300
C	0.84556700	0.18134700	0.37755400	C	0.83570500	0.09323200	-0.11175700
C	2.42913600	-1.59886800	-0.14907000	C	2.56979000	-1.61611600	0.16935400
C	1.85527200	1.13146700	0.34136700	C	1.80259800	1.09117100	-0.22272300
C	3.43668800	-0.63311400	-0.20413900	C	3.52550500	-0.60760900	0.05308500
C	3.15459900	0.72086100	0.03938700	C	3.14488800	0.73541200	-0.14080300
O	0.04972100	-1.97935600	0.24331200	O	0.17006500	-2.08884300	0.17782500
H	1.65836200	2.17725700	0.53890800	H	1.53280400	2.12902600	-0.36701100
H	-1.49986100	2.23036900	-0.23920500	H	-1.42093300	2.03398500	-0.45926500
H	-2.55952800	-2.60308600	0.18842600	H	-2.48345700	-2.80973700	0.21828200
H	2.64826600	-2.64195800	-0.33105400	H	2.86196500	-2.64610600	0.31996400
Cl	4.41425300	1.93186500	-0.01871500	Cl	4.34716300	1.99659700	-0.28390100
Cl	5.05629900	-1.16169200	-0.58342500	Cl	5.20808600	-1.05851200	0.15600000
Cl	-4.23325500	1.83250800	-0.85529200	Cl	-4.22505500	1.73636200	-0.46042800
Cl	-4.94382300	-1.23632700	-0.23644900	Cl	-4.91669600	-1.36728900	-0.04134100
C	-1.28563600	1.09844300	1.63195800	C	-2.40984000	2.77617800	2.02207800
H	-1.77532800	0.89415200	2.57543300	H	-3.22035200	2.19435200	2.53934400
		TS6				TS7	
C	-2.86950700	0.85230500	0.02244900	C	-2.91630900	0.83010700	0.07403000
C	-1.64670400	1.22144100	0.45045200	C	-1.63709500	1.23562200	0.35707400
C	-0.69116100	0.21205800	0.94128900	C	-0.67491800	0.34587800	0.91999700
C	-1.11703600	-1.30875800	0.77332600	C	-1.14294400	-1.41564000	0.71683300
C	-2.41032900	-1.57514700	0.13951600	C	-2.36411400	-1.57929400	0.00919700
C	-3.25293200	-0.55878700	-0.13496100	C	-3.26903300	-0.55339100	-0.10039100
C	1.05949200	-1.17711200	0.19188400	C	1.06056600	-1.14714600	0.23039000
C	0.75221300	0.14837900	0.53677800	C	0.74646700	0.19981600	0.51748900
C	2.32975700	-1.55126100	-0.20825400	C	2.33752700	-1.53557700	-0.13341900
C	1.73284900	1.12336500	0.45976200	C	1.74501700	1.16051900	0.39968000
C	3.31300900	-0.56088000	-0.28018300	C	3.32829000	-0.55844700	-0.23729300
C	3.02021100	0.76888600	0.04627400	C	3.03402100	0.78700800	0.02113600
O	0.00317900	-2.04744700	0.25920600	O	0.02216600	-2.05767800	0.25900500

H	1.52646900	2.15410600	0.71837600	H	1.53910500	2.20098800	0.61552800
H	-1.34530200	2.26079100	0.39927000	H	-1.32209200	2.22693400	0.05028200
H	-2.67076100	-2.59741900	-0.10565100	H	-2.54846600	-2.52334500	-0.49004000
H	2.55718100	-2.57518100	-0.47106100	H	2.55918600	-2.57115000	-0.35232600
Cl	4.24048000	2.01894700	-0.03776700	Cl	4.25957500	2.02681500	-0.10025300
Cl	4.91330400	-1.03284700	-0.79613500	Cl	4.93164500	-1.06017100	-0.70747000
Cl	-3.99746300	2.09659200	-0.47798700	Cl	-4.07042200	2.07243100	-0.38474100
Cl	-4.83016300	-0.93764000	-0.79211000	Cl	-4.85072100	-0.95702000	-0.74475700
C	-0.99486100	-0.68395500	2.06471700	C	-1.01202000	-0.66104200	1.93235200
H	-0.98773200	-0.79181900	3.13511700	H	-0.40909900	-0.91743500	2.79483800
		TS8				TS9	
C	-2.88513500	0.83851400	0.05402600	C	-2.94020400	0.80168200	0.02341800
C	-1.62948400	1.24393000	0.38564000	C	-1.59912200	1.29371100	0.14160200
C	-0.67213200	0.29091200	0.90881500	C	-0.64986300	0.56638400	0.80889100
C	-1.11853100	-1.37770500	0.72187800	C	-1.18576800	-1.52551400	0.62641000
C	-2.36756400	-1.59686700	0.04359400	C	-2.31274400	-1.61923000	-0.13390200
C	-3.24704500	-0.56754300	-0.11765300	C	-3.26755100	-0.54974200	-0.10889600
C	1.07819600	-1.16443100	0.21627000	C	1.05076900	-1.08703500	0.24128600
C	0.75426000	0.16990500	0.50044200	C	0.75995200	0.29135200	0.44162800
C	2.36031400	-1.55246000	-0.13045300	C	2.33972100	-1.50844100	-0.04668000
C	1.73660200	1.14355600	0.39299300	C	1.79850000	1.21066200	0.30881900
C	3.34170900	-0.56523300	-0.22714800	C	3.36136300	-0.56969700	-0.16580600
C	3.03290600	0.77776800	0.02523600	C	3.09125600	0.79370700	0.00398900
O	0.02497300	-2.04391700	0.25124700	O	0.04637200	-2.04629900	0.23584600
H	1.52192900	2.18298900	0.60500400	H	1.60767400	2.26421900	0.46721900
H	-1.33083300	2.26811000	0.19550400	H	-1.33463800	2.15353200	-0.46601000
H	-2.59075300	-2.57862400	-0.35594000	H	-2.43240200	-2.39932500	-0.87748200
H	2.59338500	-2.58707700	-0.34140700	H	2.54091800	-2.56042600	-0.19776400
Cl	4.24755700	2.02952000	-0.09344900	Cl	4.34867800	1.99839000	-0.13690600
Cl	4.95505100	-1.05231600	-0.68382400	Cl	4.96799700	-1.13810500	-0.53958400
Cl	-4.04464500	2.06975600	-0.41239100	Cl	-4.16070500	2.02835800	-0.28974400
Cl	-4.82922700	-0.95468300	-0.76155400	Cl	-4.89763400	-1.00153700	-0.58592300
C	-1.06433800	-0.64082400	1.96325200	C	-1.11642100	-0.52306800	1.66482300
H	-1.90056100	-0.49989800	2.63622300	H	-1.12357000	-0.61702800	2.74044800
		TS10				TS11	
C	-2.98875500	0.82941100	-0.09776600	C	-2.93396700	0.85133800	0.12040500
C	-1.66297200	1.21879600	0.00652600	C	-1.55886800	1.15334700	0.41459700
C	-0.67177200	0.23298200	0.04542900	C	-0.63190100	0.16725100	0.51939200
C	-1.05022700	-1.12286500	-0.03559000	C	-1.01409500	-1.25772400	0.57431200
C	-2.37623100	-1.53130400	-0.14711800	C	-2.53510500	-1.60234900	0.11277500
C	-3.34565300	-0.53797400	-0.17122800	C	-3.36555200	-0.41222900	-0.14724400
C	1.14276600	-1.12290100	-0.11686800	C	1.17713000	-1.17176900	0.12141900
C	0.77767400	0.22682000	0.00666300	C	0.81042800	0.16265500	0.35809300
C	2.45523800	-1.54820000	-0.18649500	C	2.47777400	-1.54464800	-0.16668600

C	1.77424800	1.19905600	0.05537800	C	1.78286700	1.15824700	0.31136400
C	3.44223900	-0.56397600	-0.13768400	C	3.44494100	-0.53840200	-0.19749800
C	3.10468900	0.79903400	-0.01842700	C	3.10240500	0.80395200	0.04252800
O	0.04320300	-1.94878400	-0.15217800	O	0.12421600	-2.03881500	0.19099600
H	1.53781200	2.25035700	0.15298400	H	1.53629000	2.19789300	0.48331900
H	-1.41529500	2.27061100	0.05296300	H	-1.26509000	2.19511600	0.40586900
H	-2.64308400	-2.57626600	-0.22113400	H	-2.71272500	-2.45934100	-0.53634000
H	2.71496800	-2.59374700	-0.27783000	H	2.74423300	-2.57563700	-0.35388400
Cl	4.34474800	2.02875100	0.04271400	Cl	4.31269000	2.06622100	0.00835700
Cl	5.10815900	-1.07085100	-0.22993100	Cl	5.09351600	-0.99857500	-0.53651000
Cl	-4.21462800	2.06983400	-0.13642800	Cl	-3.99312300	2.23299400	-0.08103700
Cl	-5.01407400	-1.02254000	-0.29372000	Cl	-4.92352600	-0.73952400	-0.86146000
C	-1.26226300	-0.80259200	2.39792700	C	-1.99040800	-1.83660100	1.44287200
H	-0.38540200	-1.50670200	2.40118500	H	-2.21279500	-2.18489600	2.43614100
		TS12				TS13	
C	-2.90015800	0.90183800	0.12005600	C	-2.87589500	0.89378000	0.14298300
C	-1.59041300	1.21673700	0.18418100	C	-1.55761200	1.16110400	0.34178200
C	-0.58315100	0.18266300	0.21535800	C	-0.58063100	0.12748600	0.40876100
C	-0.93196900	-1.13611400	0.24720500	C	-0.93131600	-1.20303000	0.33491200
C	-2.30357000	-1.64276300	0.28370900	C	-2.23953900	-1.76300100	0.40770500
C	-3.39686800	-0.50435800	0.14911700	C	-3.47698800	-0.43725600	0.21141700
C	1.24546800	-1.15027500	0.08308400	C	1.24210500	-1.17676600	0.04684700
C	0.86090200	0.20067300	0.12373600	C	0.86072100	0.15762300	0.25664000
C	2.55816700	-1.57066000	-0.00935700	C	2.55010800	-1.57461300	-0.15447600
C	1.85143700	1.18230400	0.06202300	C	1.84397000	1.14723600	0.25414600
C	3.53443200	-0.57785200	-0.06740400	C	3.52114500	-0.57471200	-0.14946100
C	3.18151900	0.78643500	-0.03197400	C	3.16921400	0.77466200	0.05323700
O	0.14512200	-1.97178400	0.15093900	O	0.15209400	-2.00995100	0.07435400
H	1.61107000	2.23700700	0.08692300	H	1.60280700	2.19059100	0.40954000
H	-1.29530000	2.25818600	0.20810000	H	-1.23665100	2.19516700	0.33475500
H	-2.48461300	-2.56527000	-0.26943800	H	-2.38558100	-2.71874900	-0.09512400
H	2.82544600	-2.61804400	-0.03776200	H	2.81735200	-2.61044500	-0.31191000
Cl	4.41005100	2.03022800	-0.10695800	Cl	4.39034000	2.02783800	0.05835700
Cl	5.20531300	-1.07432700	-0.18582500	Cl	5.18474000	-1.04411000	-0.40145100
Cl	-4.10681700	2.16875400	0.09443900	Cl	-3.95539900	2.23720600	-0.20320800
Cl	-4.79034100	-0.86603800	-0.96034600	Cl	-4.88172600	-0.76803900	-0.84077400
C	-3.25608800	-1.29157500	1.33816800	C	-3.28014700	-1.32024600	1.32349200
H	-3.64532300	-1.51641200	2.31497100	H	-4.03070700	-1.94975700	1.78030700
		TS14				TS15	
C	-2.88950800	0.89496500	0.12783300	C	-2.85061900	0.97697600	-0.11173500
C	-1.55659900	1.11614300	0.36545200	C	-1.50712300	1.32520800	-0.01997500
C	-0.59591300	0.06877000	0.45159400	C	-0.54410700	0.32035500	-0.10633100
C	-0.93241100	-1.27255900	0.32428800	C	-0.95740700	-1.00939800	-0.28360400
C	-2.24491600	-1.79974900	0.39218600	C	-2.28485100	-1.38518600	-0.37788900

C	-3.50900200	-0.39966000	0.24846100	C	-3.23482600	-0.36698100	-0.28739100
C	1.23794900	-1.20254700	0.01143600	C	1.23136600	-1.08784700	-0.21243100
C	0.84581100	0.11587000	0.28956900	C	0.90373400	0.26869300	-0.05875300
C	2.54748500	-1.57573300	-0.22393100	C	2.53139100	-1.55698300	-0.22084100
C	1.81882800	1.11474000	0.32236600	C	1.92891700	1.20080800	0.09377700
C	3.50872500	-0.56705800	-0.18166700	C	3.54562200	-0.61299700	-0.06687600
C	3.14572800	0.76709300	0.08925400	C	3.24670900	0.75543800	0.08906200
O	0.15833400	-2.04986000	0.00977100	O	0.11018800	-1.86905300	-0.35043400
H	1.56879800	2.14679400	0.53067200	H	1.72406200	2.25637400	0.21543600
H	-1.20075000	2.13848000	0.32742300	H	-1.23440200	2.36353100	0.11605000
H	-2.50736600	-2.68787400	-0.17680300	H	-2.58008800	-2.41585400	-0.51381900
H	2.82302700	-2.59984100	-0.43474500	H	2.76030600	-2.60695200	-0.33988800
Cl	4.35374100	2.03160300	0.14205800	Cl	4.52159700	1.93641800	0.28235000
Cl	5.17354400	-1.00622800	-0.47465500	Cl	5.19701200	-1.17606000	-0.07234100
Cl	-3.87950400	2.25298400	-0.38590300	Cl	-4.04789300	2.24652600	-0.00060600
Cl	-4.95222600	-0.79191500	-0.70299100	Cl	-4.92327300	-0.81343200	-0.39743800
C	-3.17414400	-1.24725800	1.35933500	C	-3.70330500	-2.26663400	2.21021900
H	-2.98700600	-0.94632600	2.38357000	H	-4.09091800	-1.30206000	2.63890400
		TS16				TS17	
C	-2.89957400	0.81747800	-0.11168800	C	3.14450600	0.67427200	-0.09410500
C	-1.56216000	1.20386900	-0.08843100	C	1.78159300	1.14448500	-0.42656400
C	-0.57860000	0.21912900	-0.09782800	C	0.87028700	0.19408100	-1.03190000
C	-0.95683600	-1.13476800	-0.12081300	C	1.11095100	-1.11431200	-0.48029900
C	-2.26967500	-1.55104000	-0.14362500	C	2.35703800	-1.59927300	-0.20223400
C	-3.25848800	-0.55344200	-0.14473000	C	3.42555700	-0.65671700	-0.07666600
C	1.23257700	-1.14593800	-0.07760900	C	-1.03187600	-0.97725300	0.04741300
C	0.86902700	0.21005700	-0.06790200	C	-0.74096400	0.44170100	0.09560500
C	2.54582000	-1.57720500	-0.05978800	C	-2.30549100	-1.50733800	0.08836100
C	1.86853500	1.18168400	-0.03592900	C	-1.93255800	1.24884200	-0.02329600
C	3.53353800	-0.59440800	-0.02821800	C	-3.41133500	-0.66619100	0.11165200
C	3.19787300	0.77527700	-0.01613400	C	-3.20411400	0.72925900	0.02143200
O	0.13357700	-1.96788600	-0.10739400	O	0.00781300	-1.83512700	-0.15221300
H	1.63386800	2.23793100	-0.02454600	H	-1.82074200	2.32317400	-0.07651500
H	-1.31451700	2.25647700	-0.05947800	H	1.83036000	2.14131400	-0.86060700
H	-2.54259300	-2.59661000	-0.16748900	H	2.51337700	-2.63893200	0.05357100
H	2.80399500	-2.62707400	-0.06690200	H	-2.42817000	-2.58170200	0.05748100
Cl	4.44091400	2.00354900	0.02449900	Cl	-4.56101300	1.82725700	-0.03764500
Cl	5.19968500	-1.10870500	-0.00248000	Cl	-5.00237300	-1.35744500	0.18531200
Cl	-4.12216700	2.05946800	-0.14905800	Cl	4.33723100	1.89443100	0.20460600
Cl	-4.91536900	-1.04776900	-0.39943700	Cl	5.01708100	-1.27755400	0.25003000
C	-3.01939900	-0.46763100	2.30261900	C	0.47522100	1.20868000	0.54253900
H	-4.11727800	-0.23725800	2.26812400	H	0.16402800	2.24203800	0.37299700
		TS18				TS19	
C	-2.82876300	0.88958400	-0.08142400	C	-2.82733800	0.87168500	-0.06927000

C	-1.49451000	1.25037300	-0.04746500	C	-1.49207000	1.24065800	-0.03574500
C	-0.51437500	0.25046300	-0.03736600	C	-0.51181900	0.24510400	-0.03121400
C	-0.91232700	-1.09714000	-0.08501200	C	-0.90961300	-1.10711600	-0.07322700
C	-2.22987500	-1.49928200	-0.13097900	C	-2.22114300	-1.51324600	-0.10258000
C	-3.19919700	-0.48407100	-0.03953600	C	-3.19777500	-0.50016700	-0.02118300
C	1.28086100	-1.13638300	-0.06064700	C	1.28481600	-1.13934800	-0.05041100
C	0.93092300	0.22436000	-0.01995900	C	0.93313700	0.22124400	-0.01540400
C	2.58731900	-1.58350700	-0.05884200	C	2.59228200	-1.58360900	-0.05040600
C	1.94456500	1.18160900	0.02564700	C	1.94500300	1.18060000	0.02410600
C	3.58941600	-0.61363400	-0.01283700	C	3.59276700	-0.61160400	-0.01125000
C	3.26962400	0.75757400	0.02908200	C	3.27088900	0.75924100	0.02550200
O	0.16982900	-1.94475800	-0.10110100	O	0.17651500	-1.95055300	-0.08476600
H	1.72448800	2.24050200	0.05955900	H	1.72312800	2.23927100	0.05375700
H	-1.23112600	2.30002300	-0.03386800	H	-1.23264700	2.29131000	-0.02660500
H	-2.51309000	-2.54044400	-0.19433600	H	-2.50675600	-2.55509900	-0.11842000
H	2.83246800	-2.63610500	-0.09072100	H	2.83915200	-2.63591300	-0.07798000
Cl	4.52753200	1.97126900	0.08728200	Cl	4.52670700	1.97547000	0.07545000
Cl	5.24978400	-1.15069300	-0.00851100	Cl	5.25389000	-1.14550800	-0.00910400
Cl	-4.04367900	2.13502900	-0.09969500	Cl	-4.04098900	2.13035900	-0.11310900
Cl	-4.88103300	-0.96117200	-0.44148200	Cl	-4.87610400	-0.97016700	-0.45880400
C	-4.48466500	-0.77850400	1.70734200	C	-4.46423400	-0.99672200	1.68353200
H	-4.29964200	-1.87992600	1.80105600	H	-4.88395500	0.03191000	1.80732100
		TS20				TS21	
C	-2.71879800	0.91357900	0.23886400	C	-2.89402100	0.84177900	0.18810000
C	-1.38414800	1.28173400	0.13133500	C	-1.54866200	1.21830300	0.10149500
C	-0.41985900	0.27329000	0.15122100	C	-0.57506700	0.23412800	0.09278100
C	-0.82966100	-1.06306500	0.28145800	C	-0.96892000	-1.13555800	0.19529100
C	-2.15491600	-1.43984900	0.38730800	C	-2.25230300	-1.56044800	0.29138900
C	-3.13124600	-0.43294700	0.36768300	C	-3.35254500	-0.56943700	0.25884100
C	1.35918100	-1.13595800	0.15652500	C	1.23121400	-1.13950300	0.11544700
C	1.02652000	0.22546300	0.06855100	C	0.86646000	0.21645300	0.04451300
C	2.66058500	-1.60076200	0.11510700	C	2.54208700	-1.57039500	0.08814000
C	2.04660900	1.16594900	-0.06711100	C	1.86627700	1.18455400	-0.05525500
C	3.66930500	-0.64834400	-0.02105200	C	3.53126200	-0.58984600	-0.01201200
C	3.36487700	0.72475800	-0.11170500	C	3.19581000	0.77704900	-0.08260700
O	0.24392100	-1.92467500	0.28576200	O	0.13523600	-1.96176300	0.21349600
H	1.83661400	2.22507300	-0.13893000	H	1.63091200	2.23912800	-0.11294200
H	-1.11471800	2.32563900	0.03788800	H	-1.30132400	2.27003000	0.03893500
H	-2.43979200	-2.47976600	0.48102900	H	-2.51385000	-2.60427500	0.39908600
H	2.89473700	-2.65405800	0.18439800	H	2.80123100	-2.61866200	0.14212100
Cl	4.63325400	1.91644500	-0.28346900	Cl	4.43653800	2.00102700	-0.20859700
Cl	5.32177400	-1.20685000	-0.07671900	Cl	5.19468600	-1.10770700	-0.04625200
Cl	-3.93120000	2.18512000	0.23475400	Cl	-4.10771800	2.08390400	0.05773200
Cl	-5.53593500	-1.00558300	-0.90319200	Cl	-4.64236100	-1.09631700	-1.07644200

C	-4.54788900	-0.80244700	0.50062000	C	-3.83657900	-0.37298000	1.59490700
H	-5.06573800	-0.90313000	1.44332700	H	-3.50840800	-0.77212700	2.54916700
		TS22				TS23	
C	-2.89268900	0.83376300	0.23944900	C	-2.88854100	0.84529800	0.20253800
C	-1.54796000	1.20902900	0.13623300	C	-1.57832400	1.20980000	0.09697900
C	-0.57855900	0.22361400	0.12320400	C	-0.57997000	0.20465100	0.10192500
C	-0.96652200	-1.14877000	0.24419600	C	-0.95304500	-1.13964800	0.24401700
C	-2.24309700	-1.57013500	0.37654100	C	-2.25842700	-1.57084400	0.33879400
C	-3.34742600	-0.57754800	0.31348000	C	-3.33986700	-0.57302500	0.26730500
C	1.23188800	-1.14403000	0.14712000	C	1.23627600	-1.14476400	0.16205300
C	0.86223000	0.20959900	0.06148600	C	0.85581900	0.20682600	0.05020400
C	2.54541500	-1.56919400	0.11531800	C	2.55235900	-1.56464900	0.14220000
C	1.85652400	1.18147800	-0.05855800	C	1.84828600	1.18254600	-0.08309800
C	3.52826300	-0.58578400	-0.00557300	C	3.52900800	-0.57866100	0.00876700
C	3.18685300	0.77996800	-0.09159900	C	3.17851200	0.78510800	-0.10240100
O	0.14279800	-1.96930800	0.26346500	O	0.14716200	-1.96523900	0.28703200
H	1.61527300	2.23402800	-0.12777800	H	1.60355100	2.23250900	-0.17456400
H	-1.29855200	2.25890500	0.05325000	H	-1.31486200	2.25811600	0.03618600
H	-2.50745300	-2.60670200	0.53212800	H	-2.52637100	-2.61517100	0.40239400
H	2.80971600	-2.61544200	0.18144800	H	2.82176300	-2.60829300	0.22699800
Cl	4.42158000	2.00628300	-0.24321900	Cl	4.40939100	2.01370900	-0.27081000
Cl	5.19306600	-1.09557700	-0.04651100	Cl	5.19818000	-1.07816000	-0.01593900
Cl	-4.09884100	2.07776600	0.04331700	Cl	-4.12880900	2.05792400	0.29020200
Cl	-4.56708000	-1.12413500	-1.17288100	Cl	-4.51476600	-0.93994000	-1.34686700
C	-3.85722000	-0.41919700	1.61377900	C	-3.91946700	-0.88349500	1.51487200
H	-4.55589200	0.25319300	2.09076900	H	-4.24503000	-0.33017100	2.38582000
		TS24				TS25	
C	-2.78487400	0.67504400	-0.24656600	C	-2.90018800	0.61395700	-0.02008600
C	-1.46309500	1.10452000	-0.20123500	C	-1.57001900	1.05763200	-0.09623800
C	-0.45145400	0.14893500	-0.12359900	C	-0.55395600	0.10922100	-0.03327400
C	-0.79715000	-1.21187100	-0.08890600	C	-0.88857400	-1.25416800	0.01229700
C	-2.10262500	-1.66401900	-0.12690100	C	-2.19504000	-1.71990400	-0.01870400
C	-3.10165100	-0.69598100	-0.20884600	C	-3.20838900	-0.77558800	-0.07103600
C	1.39306600	-1.16663700	0.00465100	C	1.30308400	-1.19591200	0.02717900
C	0.99665900	0.17846200	-0.06100700	C	0.89603800	0.14687700	-0.02789800
C	2.71458900	-1.56432900	0.07541200	C	2.62864300	-1.58502100	0.05251900
C	1.97255200	1.17361800	-0.05447400	C	1.86564900	1.14741900	-0.05935800
C	3.67924800	-0.55757100	0.08060200	C	3.58706000	-0.57257500	0.01974600
C	3.31104300	0.80095400	0.01639900	C	3.20840000	0.78306700	-0.03647300
O	0.31314200	-2.01646700	-0.01157400	O	0.22890900	-2.05212000	0.05151700
H	1.71414700	2.22329500	-0.10291200	H	1.59963200	2.19550700	-0.10078100
H	-1.24449400	2.16397700	-0.22652100	H	-1.36205700	2.11720800	-0.16129500
H	-2.34594500	-2.71694100	-0.09368800	H	-2.42346700	-2.77688500	-0.00879100
H	2.99714500	-2.60676900	0.12524400	H	2.91917200	-2.62559300	0.09548600

Cl	4.52317300	2.06113000	0.02372400	Cl	4.41200200	2.05111700	-0.07783200
Cl	5.35644100	-1.03055200	0.16913900	Cl	5.26939500	-1.03548300	0.04953800
Cl	-4.04989000	1.87886700	-0.34170300	Cl	-4.16443900	1.81759700	-0.47635100
Cl	-4.76332800	-1.22818100	-0.25510000	Cl	-4.85755800	-1.31665200	-0.11597100
C	-5.87364400	0.70931900	1.94153700	C	-3.92640600	1.47227200	1.67377400
H	-6.71069800	0.90400000	1.21503600	H	-3.25217100	2.36121600	1.77902500
		TS26				TS27	
C	-2.89531200	0.62315200	-0.00319700	C	-2.84908700	0.45584600	0.36494800
C	-1.55890000	1.06154500	-0.07472000	C	-1.52828300	0.92061800	0.35806800
C	-0.55030500	0.11295500	-0.03183100	C	-0.47526400	0.02582800	0.17606300
C	-0.88562400	-1.25467200	0.00996900	C	-0.76616400	-1.33637100	-0.00284800
C	-2.19012700	-1.71628300	-0.00807000	C	-2.05219500	-1.84634700	-0.00387900
C	-3.20181100	-0.76385300	-0.05608200	C	-3.08038500	-0.92754400	0.18213900
C	1.30700100	-1.19418200	0.02066700	C	1.42052700	-1.19247700	-0.09989600
C	0.90102900	0.14850700	-0.02560400	C	0.97072000	0.12031900	0.11147000
C	2.63227300	-1.58412000	0.04189100	C	2.75560600	-1.52763000	-0.21857100
C	1.86990300	1.14921300	-0.04945200	C	1.90697600	1.14824800	0.20771600
C	3.59083200	-0.57140700	0.01555100	C	3.68016500	-0.48828700	-0.11996700
C	3.21287800	0.78465900	-0.03028300	C	3.25884300	0.83884900	0.09200200
O	0.23232400	-2.05172100	0.04236600	O	0.37424600	-2.08205400	-0.17020500
H	1.60279000	2.19733100	-0.08146000	H	1.60825100	2.17562900	0.36961200
H	-1.35364700	2.12293400	-0.09494400	H	-1.34455500	1.97966300	0.49407300
H	-2.42266700	-2.77231400	-0.00020100	H	-2.25093500	-2.90061500	-0.13837600
H	2.92273400	-2.62495600	0.07779600	H	3.07827500	-2.54664100	-0.38121100
Cl	4.41660300	2.05239100	-0.06259200	Cl	4.42042900	2.14057700	0.21575500
Cl	5.27286800	-1.03522900	0.04097900	Cl	5.37444500	-0.88194600	-0.26625800
Cl	-4.16259900	1.81629300	-0.49513000	Cl	-4.80510500	2.08018700	-0.76375000
Cl	-4.85572600	-1.31979300	-0.11589900	Cl	-4.72510200	-1.53408200	0.20852000
C	-3.79422700	1.67158000	1.64765500	C	-3.95061500	1.40486600	0.58021800
H	-4.64294600	0.95594000	1.77582800	H	-4.32940600	1.69238000	1.55020300
		TS28				TS29	
C	-2.89024000	1.04152200	-0.01042900	C	-3.07533000	0.63275200	-0.09049400
C	-1.53933200	1.37938100	0.02912500	C	-1.67566600	1.20912300	0.06511500
C	-0.58342600	0.36763400	-0.01830600	C	-0.63005000	0.12063400	0.05208300
C	-1.00423100	-0.97194300	-0.09744800	C	-1.00336300	-1.20952600	0.11347000
C	-2.34307400	-1.32483900	-0.13336900	C	-2.31860800	-1.68101600	0.10036900
C	-3.29616600	-0.30348800	-0.09133500	C	-3.34437500	-0.71039600	-0.02647900
C	1.18242900	-1.05263700	-0.08582100	C	1.18605700	-1.22098800	0.07249200
C	0.86528900	0.31177300	-0.01023900	C	0.79999100	0.13627200	0.02202500
C	2.47801700	-1.53166800	-0.10392700	C	2.50054100	-1.64014100	0.05467700
C	1.89837000	1.24572000	0.05013600	C	1.79972900	1.11468000	-0.05824500
C	3.50097000	-0.58621800	-0.04256800	C	3.48140200	-0.65043800	-0.02186600
C	3.21317000	0.79171000	0.03385200	C	3.13000800	0.71459500	-0.07990700
O	0.05221300	-1.83547000	-0.13881100	O	0.09202500	-2.04058800	0.13098700

H	1.70262000	2.30830900	0.10926900	H	1.56319500	2.16912900	-0.10724200
H	-1.25645800	2.42204600	0.09239100	H	-1.49185300	1.90441100	-0.77859600
H	-2.62704300	-2.41928000	-0.45379400	H	-2.54969900	-2.73465900	0.15037200
H	2.69656900	-2.58893800	-0.16217400	H	2.76773400	-2.68714600	0.09444900
Cl	4.49855300	1.97363200	0.11107100	Cl	4.36264600	1.95069800	-0.18362300
Cl	5.14790600	-1.15870700	-0.06288300	Cl	5.15205300	-1.15118800	-0.04761200
Cl	-4.06703700	2.33218200	0.04539700	Cl	-4.31910800	1.82005500	-0.29270900
Cl	-4.98126100	-0.72930800	-0.15014200	Cl	-4.98458600	-1.31185900	-0.11849100
C	-2.77856600	-3.27239300	0.65396600	C	-1.53228600	2.01704600	1.31776700
H	-3.32138100	-2.70828200	1.44442500	H	-0.52095500	2.44639200	1.38846800
TS30							
C	-2.96098400	0.89224800	0.04419200				
C	-1.61039000	1.21522600	0.26590000				
C	-0.68679800	0.21093800	0.40977000				
C	-1.12130100	-1.21368900	0.52428000				
C	-2.44625000	-1.49101400	-0.04797000				
C	-3.34587000	-0.46600000	-0.16947500				
C	1.12509500	-1.13543300	0.01172000				
C	0.74883900	0.19265300	0.27812300				
C	2.42657300	-1.50854500	-0.24388100				
C	1.72849800	1.18350800	0.28836500				
C	3.40081700	-0.50411100	-0.22241100				
C	3.05413900	0.83132100	0.04421400				
O	0.05547100	-2.01089900	-0.01864100				
H	1.48200400	2.21786100	0.48901500				
H	-1.31200300	2.25601900	0.24450600				
H	-2.74543400	-2.51731800	-0.21398900				
H	2.69370700	-2.53505000	-0.45301000				
Cl	4.26677400	2.08811500	0.07848500				
Cl	5.05306300	-0.96123200	-0.53094100				
Cl	-4.11241100	2.18427100	-0.08307600				
Cl	-4.99202700	-0.84667500	-0.62178000				
C	-0.79655900	-1.92847800	1.81819600				
H	-1.31868800	-2.90220900	1.75074800				
IM1-F				IM2-F			
C	-3.06525900	0.79015400	-0.00291200	C	-3.06856900	0.80772200	-0.00196900
C	-1.58118800	1.31365300	0.13362400	C	-1.59495300	1.32216400	0.11062500
C	-0.55073700	0.26310800	0.12426000	C	-0.54788200	0.28191800	0.09897200
C	-0.89771700	-1.05900000	0.13675300	C	-0.90452700	-1.03806700	0.10904500
C	-2.23105200	-1.57060700	0.06803700	C	-2.24250300	-1.54546700	0.04304000
C	-3.23325800	-0.68094300	-0.03231200	C	-3.24964700	-0.65512000	-0.04822500
C	1.28595400	-1.05244100	0.04356200	C	1.27990300	-1.04567500	0.02909400
C	0.88484500	0.29842500	0.03763500	C	0.88733000	0.30834900	0.02496100
C	2.60945200	-1.46105600	0.00091700	C	2.60117500	-1.46244200	-0.00728500

C	1.86440300	1.29957800	-0.01783200	C	1.87367800	1.30366000	-0.02139600
C	3.55395400	-0.44991400	-0.05935200	C	3.55214900	-0.45696300	-0.05789500
C	3.18639600	0.90300900	-0.06940700	C	3.19321300	0.89860300	-0.06568400
O	0.19926100	-1.88348100	0.10559600	O	0.18793900	-1.86983700	0.08240400
H	1.62534500	2.35540300	-0.01828200	H	1.64064000	2.36080700	-0.02051800
H	-1.34312000	2.22522300	-0.41488400	H	-1.40757600	2.22894200	-0.46552200
H	-2.42846300	-2.63432800	0.07346800	H	-2.43923200	-2.60945200	0.04143100
H	2.90715300	-2.50094500	0.00817400	H	2.89245600	-2.50416100	-0.00241500
C	-2.61375200	1.48596000	1.18385400	C	-2.57642400	1.46208500	1.20216100
H	-2.98598600	2.39365200	1.63517300	H	-2.59417500	1.21993500	2.25485700
F	4.16440800	1.82881400	-0.12580600	F	4.17764500	1.81779800	-0.11269300
F	4.86235500	-0.76148500	-0.10965400	F	4.85879500	-0.77636300	-0.10083300
F	-4.50765900	-1.09020400	-0.16285000	F	-4.52258300	-1.07013000	-0.17533900
F	-3.92368900	1.43946300	-0.86940000	F	-3.93755400	1.49291900	-0.82888300
		IM3-F				IM5-F	
C	-3.04515900	0.79075400	-0.27361500	C	-2.82279900	1.00611800	-0.16358100
C	-1.76567000	1.40866900	0.08006400	C	-1.61027100	1.40710600	0.25474000
C	-0.61882800	0.32775000	0.51205800	C	-0.67318100	0.39436900	0.75814100
C	-1.01924400	-1.08657600	0.35470100	C	-1.10398300	-1.17229900	0.56385200
C	-2.28015000	-1.51157700	0.14991700	C	-2.37392300	-1.43170300	-0.10235400
C	-3.29518400	-0.52884300	-0.12735700	C	-3.19658000	-0.39236800	-0.33907500
C	1.18325800	-1.04666200	0.10543200	C	1.08978000	-1.01771000	0.05638600
C	0.83660900	0.30178600	0.20797200	C	0.77041300	0.30780400	0.37566900
C	2.48186700	-1.47798700	-0.10614800	C	2.37364700	-1.40698700	-0.29576000
C	1.81983000	1.27900600	0.11432000	C	1.75319800	1.28863500	0.31660800
C	3.44855200	-0.48678700	-0.21435400	C	3.34089900	-0.41282700	-0.34631000
C	3.12578400	0.86625900	-0.10788800	C	3.03798200	0.91433000	-0.05163200
O	0.09965200	-1.88816900	0.24302000	O	0.02602500	-1.88289500	0.08516400
H	1.60493000	2.33626900	0.20777400	H	1.55523300	2.32576400	0.55714900
H	-1.46608000	2.27225100	-0.51161500	H	-1.32561900	2.44916600	0.16983500
H	-2.52545300	-2.55795800	0.02621900	H	-2.64188900	-2.43456600	-0.41144000
H	2.74767100	-2.52316200	-0.18911700	H	2.62242200	-2.43112300	-0.53911300
C	-1.27013700	1.24677300	1.44438200	C	-1.03862500	-0.51248800	1.85930500
H	-1.77634700	1.09182100	2.38721700	H	-1.83592900	-0.39018400	2.58028100
F	4.10987000	1.77960300	-0.21801900	F	4.01602700	1.83996000	-0.11606200
F	4.72956600	-0.83253600	-0.42860200	F	4.60042800	-0.73123800	-0.69477500
F	-4.52608700	-1.00742400	-0.40948800	F	-4.41450800	-0.59574400	-0.87257400
F	-3.97902800	1.61488200	-0.79961800	F	-3.74214200	1.89949200	-0.57813900
		IM6-F				IM7-F	
C	-2.87317700	1.06735900	-0.01885800	C	-2.80763600	1.10177700	0.01475000
C	-1.51333200	1.36721300	0.31824300	C	-1.51111400	1.41999700	0.13889600
C	-0.59732400	0.36762900	0.40893700	C	-0.52332700	0.36587100	0.15271600
C	-1.00757000	-1.05226700	0.39839700	C	-0.90283100	-0.94462200	0.10220300
C	-2.50743200	-1.37888800	-0.07123500	C	-2.27574500	-1.43440700	0.07958200

C	-3.31097200	-0.17999800	-0.31045700	C	-3.34677500	-0.27875100	-0.03863400
C	1.18845400	-0.99410300	-0.00895500	C	1.27813400	-0.99691400	-0.02316600
C	0.84698200	0.33769700	0.28015300	C	0.92104100	0.35845800	0.09150500
C	2.48677700	-1.39007100	-0.29303700	C	2.58676600	-1.44428700	-0.11499900
C	1.84093600	1.31916200	0.29278600	C	1.93039500	1.32863400	0.10829700
C	3.45726200	-0.39914400	-0.26070600	C	3.56341700	-0.46291100	-0.09278000
C	3.14223000	0.93178800	0.02934900	C	3.23950800	0.89645600	0.01556500
O	0.11467900	-1.84061700	-0.00217100	O	0.16225000	-1.79646800	-0.02617200
H	1.62885900	2.35984700	0.50320200	H	1.72547600	2.38835200	0.19148400
H	-1.23161600	2.41277700	0.34681000	H	-1.22527800	2.46178700	0.21293400
H	-2.67917200	-2.21948600	-0.74223900	H	-2.44604500	-2.34271600	-0.49750800
H	2.74912600	-2.41416900	-0.52147800	H	2.84985300	-2.48995000	-0.20040100
C	-1.99209200	-1.64253400	1.27997800	C	-3.30408400	-1.14697100	1.11541000
H	-2.35006700	-1.44678700	2.28044400	H	-4.05570800	-1.81293300	1.51213400
F	4.13548400	1.84239100	0.04658300	F	4.24575900	1.79293700	0.02879100
F	4.73870400	-0.71921700	-0.50708500	F	4.86084700	-0.81085000	-0.17756200
F	-4.51105400	-0.36638600	-0.89687400	F	-4.37592600	-0.41920000	-0.94796800
F	-3.69635700	2.12206500	-0.21117400	F	-3.75654700	2.05858400	-0.04829900
		IM8-F				P1-F	
C	-2.82912500	1.08246400	-0.00520100	C	-3.54214100	0.68698900	-0.00017700
C	-1.52847600	1.40207600	0.10730200	C	-1.22340400	1.66314100	-0.00005600
C	-0.53311900	0.35078100	0.12113800	C	-0.41391500	0.47352200	-0.00003000
C	-0.90151600	-0.96295100	0.06777900	C	-0.87110000	-0.85140600	-0.00002100
C	-2.28435300	-1.44002200	0.05057900	C	-2.15431100	-1.41596100	0.00054700
C	-3.34984000	-0.29892800	-0.03535300	C	-3.34358500	-0.68005200	0.00016500
C	1.27986600	-1.00019200	-0.03227400	C	1.33385500	-0.97600800	-0.00036100
C	0.91195700	0.35345600	0.07177700	C	1.02147600	0.39319100	-0.00026900
C	2.59201300	-1.43925200	-0.11109800	C	2.62102200	-1.47934000	-0.00033900
C	1.91481400	1.33035300	0.09117800	C	2.06903300	1.32685000	0.00010300
C	3.56190900	-0.45123000	-0.08595200	C	3.63766800	-0.53350900	-0.00008800
C	3.22762400	0.90638600	0.01208100	C	3.36283700	0.83998600	0.00013800
O	0.16888100	-1.80758700	-0.04073500	O	0.18455800	-1.72458300	-0.00018200
H	1.70245400	2.38925000	0.16575900	H	1.90565900	2.39678300	0.00018400
H	-1.24322100	2.44485000	0.17082200	H	-0.68469100	2.60423500	0.00003500
H	-2.50015400	-2.32128500	-0.55356100	H	-2.24144400	-2.49388800	0.00102100
H	2.86261400	-2.48361900	-0.18867900	H	2.84402600	-2.53762900	-0.00037200
C	-3.24354000	-1.15001200	1.13872000	C	-2.58063600	1.74218900	0.00010100
H	-3.16791600	-0.97597900	2.20199600	H	-3.03049600	2.72928000	0.00025600
F	4.22744000	1.80984100	0.02893500	F	4.40153500	1.69813700	0.00040200
F	4.86234400	-0.79073300	-0.15753800	F	4.92140500	-0.93588200	-0.00006000
F	-4.41557500	-0.47079400	-0.89519800	F	-4.46494000	-1.42571400	0.00037100
F	-3.77577600	2.04167700	-0.06670100	F	-4.83247900	1.10349600	-0.00048400
		P3-F				P4-F	
C	-2.86225400	0.95845800	-0.08011700	C	-2.82831300	1.08051500	-0.00038100

C	-1.57149900	1.48551000	0.11930800	C	-1.47836200	1.19266500	0.00006000
C	-0.61597300	0.68458500	0.73504800	C	-0.52234600	0.11232600	0.00034600
C	-1.16790700	-1.38397300	0.52474600	C	-0.78987200	-1.25726400	0.00010500
C	-2.34019600	-1.51422500	-0.20534500	C	-3.27097600	-1.42342700	0.00043000
C	-3.20521100	-0.40541200	-0.23895900	C	-3.64900000	-0.09777400	-0.00023100
C	1.06486800	-0.95458900	0.13422900	C	1.40912600	-1.07874400	-0.00047700
C	0.77825000	0.41845500	0.34532800	C	0.90890400	0.23450200	-0.00015400
C	2.35306400	-1.39403700	-0.14773700	C	2.75527900	-1.39550800	-0.00050500
C	1.81708600	1.34333500	0.21062600	C	1.81485100	1.30698700	0.00029500
C	3.36039300	-0.45204900	-0.25420400	C	3.62779400	-0.31647600	-0.00012300
C	3.09432500	0.90570800	-0.08713200	C	3.16327400	1.00608100	0.00023800
O	0.03534100	-1.87791900	0.07662000	O	0.37766300	-1.97802700	-0.00050200
H	1.64836900	2.40065500	0.37194600	H	1.50217100	2.34326900	0.00048600
H	-1.33471300	2.41604200	-0.38696400	H	-1.09426000	2.20588300	0.00017400
H	-2.52825900	-2.33720200	-0.88550200	H	-4.10886700	-2.11370900	0.00160600
H	2.56388400	-2.44285500	-0.30925200	H	3.12524500	-2.41177700	-0.00071000
C	-1.13975500	-0.39092900	1.55931600	C	-1.99510000	-1.98887100	0.00035600
H	-2.02389200	-0.23401800	2.16475600	H	-1.90957900	-3.06723500	0.00103200
F	4.10247700	1.79054600	-0.20027700	F	4.07309000	1.99969800	0.00064100
F	4.61443200	-0.84441600	-0.53527700	F	4.95531700	-0.53374800	-0.00010000
F	-4.44313800	-0.61985500	-0.73498400	F	-4.98192500	0.15194800	0.00054700
F	-3.82924500	1.83102600	-0.44708200	F	-3.53621300	2.22851400	-0.00090200
		TS2-F				TS3-F	
C	-3.17470000	0.76200300	0.04666500	C	-3.26740700	0.75276500	0.07804300
C	-1.50007400	1.37065300	0.24878300	C	-1.50228100	1.40686100	0.30610000
C	-0.53843100	0.29691200	0.21635200	C	-0.51904600	0.36682400	0.26973300
C	-0.89469500	-1.03378600	0.27391600	C	-0.90829000	-0.96680500	0.33217600
C	-2.20032700	-1.54881600	0.10715500	C	-2.20303700	-1.48335200	0.10093400
C	-3.22510700	-0.68580000	-0.08847000	C	-3.26319700	-0.65308300	-0.15311800
C	1.29102400	-1.03675400	0.11412400	C	1.27952400	-1.00724400	0.14039900
C	0.89787300	0.31298900	0.06390400	C	0.91243200	0.34916300	0.07807300
C	2.61135300	-1.45392600	0.05189800	C	2.59123400	-1.44972600	0.06515000
C	1.87877000	1.30544800	-0.05675900	C	1.90937900	1.32149400	-0.06882000
C	3.55861200	-0.45203600	-0.07983000	C	3.55471500	-0.46779500	-0.09574500
C	3.19752100	0.90088700	-0.13466100	C	3.21879700	0.89116600	-0.16381200
O	0.20547100	-1.86017800	0.24251600	O	0.18322200	-1.81032600	0.29661800
H	1.64511100	2.36209700	-0.08661400	H	1.69342300	2.38164000	-0.10594900
H	-1.21855800	2.29519800	-0.25600200	H	-1.37660300	2.31060000	-0.28663400
H	-2.36940600	-2.61400700	0.01951000	H	-2.32914400	-2.54900200	-0.04373900
H	2.90411800	-2.49431200	0.09513900	H	2.86522300	-2.49476800	0.11777900
C	-2.63407800	1.47123300	1.16546400	C	-2.61236800	1.31844600	1.22955700
H	-3.03964900	2.40613000	1.52867700	H	-2.58121900	0.85941300	2.21206000
F	4.17663700	1.81899900	-0.25780200	F	4.21301500	1.78807200	-0.31535200
F	4.86299200	-0.77367500	-0.15666400	F	4.85091000	-0.81529000	-0.18948700

F	-4.42503300	-1.16099400	-0.48318300	F	-4.37684500	-1.17517100	-0.71512000
F	-4.07813100	1.41258900	-0.74813800	F	-4.11821300	1.50266100	-0.66654000
		TS4-F				TS8-F	
C	-3.06107400	0.79573900	-0.27725600	C	-2.83236600	0.99883500	-0.13599900
C	-1.81120900	1.43959900	0.08746300	C	-1.60534200	1.41837500	0.24085100
C	-0.60039300	0.33390100	0.54389700	C	-0.66377500	0.43699900	0.76257400
C	-1.01364500	-1.06531300	0.38648500	C	-1.11119300	-1.21427600	0.55605800
C	-2.28444800	-1.49062600	0.20918300	C	-2.35869700	-1.44241500	-0.13788900
C	-3.30055500	-0.52636300	-0.09043600	C	-3.19617500	-0.39569600	-0.32219000
C	1.18276500	-1.04327800	0.09593500	C	1.09143800	-1.01174300	0.07457400
C	0.84739900	0.30627900	0.23073500	C	0.76854800	0.31977900	0.37045500
C	2.47638100	-1.47970800	-0.13787100	C	2.37820500	-1.40705800	-0.26085300
C	1.83855400	1.27842200	0.14956300	C	1.75517700	1.29771100	0.29144200
C	3.44873100	-0.49376500	-0.23481800	C	3.34662700	-0.41622900	-0.32672900
C	3.13775800	0.85996800	-0.09441800	C	3.04101700	0.91705700	-0.06270200
O	0.09531900	-1.87627200	0.23220400	O	0.03232200	-1.88524800	0.08754500
H	1.63262700	2.33495100	0.26766700	H	1.55695300	2.33895700	0.51297700
H	-1.51069800	2.29796600	-0.51091300	H	-1.32083900	2.45202400	0.08112400
H	-2.52664500	-2.53993500	0.10347700	H	-2.60589800	-2.42120200	-0.53092200
H	2.73361600	-2.52485900	-0.24478900	H	2.62570700	-2.43594000	-0.48480500
C	-1.28246300	1.26482700	1.43088700	C	-1.06566700	-0.49851900	1.81320700
H	-1.77432900	1.12053300	2.38372000	H	-1.90804500	-0.36285000	2.47970800
F	4.12914800	1.76668300	-0.19343200	F	4.01878000	1.84138900	-0.14113100
F	4.72499100	-0.84348000	-0.46976100	F	4.60767400	-0.74198400	-0.66197500
F	-4.52102500	-1.02167400	-0.39157800	F	-4.41159000	-0.59947700	-0.86423600
F	-3.97577100	1.56996400	-0.90666100	F	-3.75855700	1.88830300	-0.54768300
		TS11-F				TS13-F	
C	-2.86347200	1.06261800	0.03790900	C	-2.79128700	1.10046000	-0.01021200
C	-1.52312100	1.32546700	0.42864500	C	-1.48658600	1.37389300	0.20008600
C	-0.59873200	0.31857500	0.48396100	C	-0.52496600	0.32038900	0.27112600
C	-0.98523400	-1.09077100	0.45004300	C	-0.89894300	-0.99959800	0.15527900
C	-2.57413100	-1.38595800	-0.09562800	C	-2.22256600	-1.54179300	0.15208700
C	-3.31041000	-0.16762800	-0.34151200	C	-3.42132800	-0.21631800	0.00717400
C	1.20089700	-1.01062700	0.02880000	C	1.28465600	-1.00974900	-0.05167300
C	0.84321000	0.31493400	0.32180900	C	0.91955900	0.32824700	0.17128600
C	2.49579300	-1.38964900	-0.28983900	C	2.59486300	-1.43274500	-0.21401700
C	1.82218200	1.31199000	0.30611300	C	1.91770000	1.30764000	0.22550400
C	3.45133800	-0.38425300	-0.28349900	C	3.56190400	-0.44331700	-0.15204300
C	3.12189800	0.94247600	0.01166100	C	3.22822000	0.90066200	0.06231200
O	0.13759900	-1.87181600	0.08037000	O	0.18074900	-1.82180400	-0.08052800
H	1.60044200	2.35070500	0.51609200	H	1.70382500	2.35564900	0.39272400
H	-1.23301800	2.36646800	0.50620200	H	-1.17551500	2.41134700	0.20498100
H	-2.73702300	-2.20699300	-0.79241300	H	-2.35512400	-2.47391500	-0.39646700
H	2.76719000	-2.41061000	-0.52174100	H	2.86596400	-2.46622700	-0.38224100

C	-2.03971700	-1.68170200	1.23018100	C	-3.30168500	-1.16382800	1.06846800
H	-2.40639700	-1.55087100	2.23912200	H	-4.09322400	-1.83911600	1.36378200
F	4.10108400	1.86820000	0.00074000	F	4.22491500	1.80669700	0.10940600
F	4.73148600	-0.68441700	-0.56137600	F	4.85916300	-0.76881100	-0.30065400
F	-4.43308700	-0.27331500	-1.08565800	F	-4.49321600	-0.31737300	-0.83315200
F	-3.65892600	2.13764400	-0.16727100	F	-3.65188000	2.10649000	-0.29235700
TS14-F							
C	-2.81833800	1.08794000	-0.05964700				
C	-1.49681500	1.30933400	0.20550100				
C	-0.54832200	0.25201300	0.32160600				
C	-0.89456400	-1.08467400	0.16598200				
C	-2.21737500	-1.59715900	0.16646500				
C	-3.47413800	-0.17713900	0.04169800				
C	1.28660300	-1.02989100	-0.07711400				
C	0.89783200	0.28856000	0.20917200				
C	2.60237800	-1.41734400	-0.27696900				
C	1.87614400	1.28523900	0.28997500				
C	3.55037700	-0.41140600	-0.18645500				
C	3.19273900	0.91430900	0.09072900				
O	0.20057800	-1.86632400	-0.12622000				
H	1.64332300	2.32014800	0.50658100				
H	-1.14890300	2.33483600	0.16029300				
H	-2.47525400	-2.44983300	-0.45799900				
H	2.89153100	-2.43661600	-0.49462900				
C	-3.18032900	-1.07987400	1.12170700				
H	-3.00164100	-0.81439400	2.15774200				
F	4.17071900	1.83872600	0.16361400				
F	4.85124600	-0.70329700	-0.36750700				
F	-4.57079600	-0.37094500	-0.73051200				
F	-3.58126100	2.11740600	-0.50316500				
Species	x	y	z	Species	x	y	z
IM1-Br				IM2-Br			
C	-3.11547300	0.64130200	0.37329800	C	-3.11773400	0.63877800	0.36691500
C	-1.60400800	1.10163000	0.53137500	C	-1.61129400	1.10587200	0.50509100
C	-0.60902000	0.03330500	0.34691400	C	-0.60439900	0.04691900	0.32654500
C	-1.00531700	-1.26359500	0.18596900	C	-1.00291700	-1.25230600	0.17810800
C	-2.35725400	-1.71884000	0.11392200	C	-2.35506200	-1.71147900	0.10378800
C	-3.35810400	-0.81225900	0.17066000	C	-3.36337800	-0.80877000	0.15546400
C	1.17193700	-1.31715700	0.01225700	C	1.17560700	-1.30964400	0.01111800
C	0.82180700	0.03251700	0.21188800	C	0.82675800	0.04227700	0.19821200
C	2.47558600	-1.75083600	-0.13768500	C	2.47903600	-1.74644800	-0.13145000
C	1.83771700	0.99223800	0.25859300	C	1.84386800	1.00092100	0.24081400
C	3.47592200	-0.77966000	-0.09428800	C	3.48063200	-0.77634100	-0.09246500
C	3.15669700	0.58045700	0.10068100	C	3.16281700	0.58581800	0.09062700

O	0.05883000	-2.11305400	-0.00319100	O	0.06139100	-2.10412600	-0.00134800
H	1.61661500	2.03951400	0.41570100	H	1.62338300	2.04961200	0.38902200
H	-1.34947200	2.06488300	0.09071500	H	-1.39539700	2.07075100	0.05062800
H	-2.56231800	-2.77596200	0.00964000	H	-2.55438100	-2.76939700	-0.00375500
H	2.71325600	-2.79504200	-0.28660100	H	2.71566900	-2.79208000	-0.27174000
C	-2.58938200	1.13624600	1.62443400	C	-2.56768600	1.10467200	1.61971800
H	-2.90834300	1.89339300	2.32360500	H	-2.59423800	0.72926300	2.63214600
Br	4.50932800	1.92936800	0.16584100	Br	4.51731900	1.93283500	0.15047500
Br	5.27592200	-1.37323200	-0.30951400	Br	5.28035800	-1.37431600	-0.29698700
Br	-5.16416100	-1.42102200	0.10322700	Br	-5.16393800	-1.42659500	0.06718800
Br	-4.27214700	1.87133000	-0.66571400	Br	-4.30127200	1.89731200	-0.61268800
IM3-Br				IM5-Br			
C	-3.09185900	0.61277200	0.07663700	C	-2.90403800	0.66311700	0.21346700
C	-1.77651600	1.16785100	0.44982700	C	-1.65976500	1.05951900	0.56491000
C	-0.63578500	0.05968800	0.79624000	C	-0.69763800	0.08898400	1.09179100
C	-1.06667200	-1.32827300	0.55566100	C	-1.12225500	-1.47712700	0.98566400
C	-2.33909200	-1.72059400	0.35767200	C	-2.40700500	-1.76161700	0.36788400
C	-3.36544800	-0.71467800	0.16557700	C	-3.27736900	-0.75435600	0.11414100
C	1.13103600	-1.31469800	0.26617800	C	1.05639100	-1.34329400	0.41649600
C	0.81218900	0.03010600	0.46452800	C	0.73795800	-0.00532200	0.68053600
C	2.41422100	-1.74723500	-0.00300700	C	2.33097400	-1.73556300	0.04809000
C	1.81168700	0.98666300	0.40858200	C	1.71173400	0.96996700	0.54449000
C	3.41679700	-0.77391700	-0.07591000	C	3.30892200	-0.74528600	-0.08303600
C	3.12078400	0.58151200	0.12654000	C	3.00418300	0.60012500	0.15640500
O	0.03352900	-2.14243400	0.37152700	O	0.00046000	-2.21076500	0.51977000
H	1.59923700	2.03434400	0.57732700	H	1.49316000	2.01142000	0.74158100
H	-1.44674600	2.05753900	-0.08128500	H	-1.35479800	2.08902100	0.42245600
H	-2.58055500	-2.75961000	0.18323200	H	-2.64700100	-2.78651300	0.11352200
H	2.63795400	-2.79378500	-0.15640700	H	2.55988300	-2.77411700	-0.14660200
C	-1.27385600	0.91658700	1.79512400	C	-1.03100700	-0.76038500	2.24723100
H	-1.77733600	0.69131200	2.72530900	H	-1.80328200	-0.60538000	2.98844400
Br	4.46066300	1.93887900	0.04070900	Br	4.30502100	1.98785000	-0.01087300
Br	5.18450600	-1.37611400	-0.46165500	Br	5.05404400	-1.30967000	-0.60756600
Br	-5.11594700	-1.41103700	-0.15578800	Br	-5.00700200	-1.24111800	-0.53997800
Br	-4.34767100	1.91612700	-0.52390200	Br	-4.13944000	2.01891300	-0.33775400
IM6-Br				IM7-Br			
C	-2.98437700	0.61774600	0.23541000	C	-2.96330800	0.69534300	0.24797600
C	-1.60585500	0.96330400	0.49145400	C	-1.65747500	1.03109800	0.28039900
C	-0.66300200	-0.00114900	0.64879800	C	-0.63765300	0.01348600	0.36161900
C	-1.03149700	-1.41929300	0.79870000	C	-0.97589100	-1.30214300	0.49099800
C	-2.52932700	-1.81067400	0.40689500	C	-2.33449000	-1.82252800	0.58286600
C	-3.39648300	-0.66811300	0.06466700	C	-3.44481200	-0.70842700	0.36565900
C	1.14759200	-1.35379000	0.31657500	C	1.19714100	-1.31313100	0.27016700
C	0.77840000	-0.00815200	0.47574500	C	0.80322600	0.03484300	0.23259700

C	2.44677300	-1.73824800	0.03624000	C	2.51038800	-1.73013100	0.17251600
C	1.74645900	0.98547600	0.35822100	C	1.78431900	1.01606800	0.08133600
C	3.41106600	-0.73212500	-0.06570300	C	3.47905500	-0.73700900	0.02478800
C	3.06620400	0.62089800	0.09634500	C	3.11644100	0.62394800	-0.02079600
O	0.09963200	-2.21994400	0.44856400	O	0.10507600	-2.13545600	0.41949700
H	1.49201800	2.03127200	0.46981200	H	1.53066800	2.06708100	0.04374000
H	-1.32613100	2.00559400	0.41226200	H	-1.37188600	2.07471000	0.24421200
H	-2.67608300	-2.73073400	-0.15487800	H	-2.49449100	-2.79253200	0.11431600
H	2.70991800	-2.77913300	-0.09044200	H	2.77977400	-2.77667500	0.20733200
C	-1.98418400	-1.91939100	1.76654100	C	-3.31248100	-1.41940200	1.61288200
H	-2.32306900	-1.60404600	2.74306900	H	-3.99219600	-1.98106600	2.23424900
Br	4.35955100	2.02034200	-0.03319000	Br	4.42212100	2.00438500	-0.22457500
Br	5.20148000	-1.27853100	-0.42502500	Br	5.29580100	-1.30450600	-0.11005900
Br	-5.09747500	-1.14269900	-0.64727700	Br	-4.93780700	-1.22613400	-0.83087900
Br	-4.15167900	2.10425000	-0.05872600	Br	-4.28523600	2.07482700	0.18214600
	IM8-Br				P1-Br		
C	-2.96576400	0.69190000	0.22615600	C	-3.55191400	0.77938500	-0.00033100
C	-1.65583700	1.02113700	0.25844500	C	-1.15774700	1.65581100	-0.00064700
C	-0.63668200	-0.00033000	0.33789100	C	-0.38366400	0.45015900	-0.00062400
C	-0.97231200	-1.31945600	0.44845800	C	-0.90267000	-0.85086100	-0.00056800
C	-2.33709000	-1.82757700	0.53910700	C	-2.20598500	-1.35608000	-0.00070900
C	-3.43949700	-0.70962500	0.35519300	C	-3.39798000	-0.59856100	-0.00030500
C	1.20189900	-1.32273600	0.24475100	C	1.29471200	-1.07522800	-0.00025700
C	0.80477200	0.02477100	0.21594800	C	1.04489700	0.30653700	-0.00036300
C	2.51655000	-1.73597500	0.15041800	C	2.55640500	-1.62852900	-0.00005200
C	1.78463900	1.00930100	0.07746600	C	2.13552900	1.18394000	-0.00032700
C	3.48378400	-0.73956400	0.01615500	C	3.63679200	-0.73916500	0.00001700
C	3.11813700	0.62093600	-0.02069900	C	3.42287900	0.65310600	-0.00012100
O	0.11096100	-2.14892900	0.38028300	O	0.11398200	-1.77304000	-0.00033700
H	1.52892400	2.06002900	0.04622500	H	1.99898600	2.25700600	-0.00043400
H	-1.36497400	2.06317600	0.21833100	H	-0.59368700	2.58274900	-0.00080700
H	-2.53518200	-2.78131800	0.05437500	H	-2.29399500	-2.43303000	-0.00088100
H	2.78795400	-2.78223000	0.17766100	H	2.70990900	-2.69854000	0.00003700
C	-3.26342800	-1.40879900	1.60525500	C	-2.51018900	1.78547900	-0.00053400
H	-3.18594100	-1.09950500	2.63693300	H	-2.88447500	2.80132100	-0.00059900
Br	4.42170300	2.00575100	-0.20714700	Br	4.87899600	1.89051200	0.00002500
Br	5.30250100	-1.30176200	-0.11285200	Br	5.38570200	-1.49744200	0.00037600
Br	-4.98690400	-1.24107900	-0.76800900	Br	-4.95495800	-1.72221900	0.00007700
Br	-4.27882800	2.07730100	0.14792100	Br	-5.30216900	1.56568800	0.00050200
	P3-Br				P4-Br		
C	-2.94450500	0.62984200	0.18744300	C	-2.93702300	0.41990500	0.02197200
C	-1.62115200	1.14337100	0.31445700	C	-1.57735800	0.54728300	0.03055500
C	-0.65461800	0.39763700	0.96347600	C	-0.57520200	-0.48556500	0.02277100
C	-1.18077500	-1.67243800	0.83443500	C	-0.77784700	-1.86173700	0.03854100

C	-2.34403800	-1.81850400	0.10884200	C	-3.24962600	-2.10859600	0.02815200
C	-3.27370200	-0.74095500	0.08281300	C	-3.72356300	-0.79337100	0.00332900
C	1.04416900	-1.24321500	0.41250500	C	1.40775000	-1.58946900	0.02388600
C	0.74372500	0.13213300	0.57673400	C	0.85183600	-0.30062900	0.01303400
C	2.33338600	-1.66911800	0.13361200	C	2.76281300	-1.84344400	0.01921500
C	1.77020400	1.05688500	0.40274200	C	1.71518400	0.80103200	-0.00339100
C	3.34790700	-0.72630300	-0.02073100	C	3.61244000	-0.73370200	0.00272900
C	3.06598400	0.63994600	0.10363700	C	3.08865800	0.57502300	-0.00832000
O	0.02883100	-2.18424600	0.41458200	O	0.41496900	-2.53417100	0.03989500
H	1.56817200	2.11223600	0.53084900	H	1.33984200	1.81560100	-0.01298000
H	-1.37278100	2.03517700	-0.25087900	H	-1.19299700	1.55877700	0.04846400
H	-2.49729500	-2.66009200	-0.55624100	H	-4.03001400	-2.86090700	0.02597000
H	2.53503800	-2.72488700	0.01407200	H	3.15428600	-2.85098500	0.02789900
C	-1.15201600	-0.64724300	1.84264500	C	-1.96057800	-2.62608200	0.05142800
H	-2.01484500	-0.48223600	2.47548500	H	-1.84479800	-3.70208400	0.07089200
Br	4.40535300	1.98315900	-0.10081100	Br	4.22830400	2.10834700	-0.03104800
Br	5.09680500	-1.37285700	-0.41540000	Br	5.48788400	-1.07551700	-0.00398200
Br	-5.04388600	-1.25944000	-0.45843400	Br	-5.63977500	-0.67378000	-0.07057700
Br	-4.26559500	1.97203900	-0.20208500	Br	-3.86415500	2.10692400	0.05009700
		TS2-Br				TS3-Br	
C	-3.22798300	0.63031000	0.50511000	C	-3.29350900	0.61491500	0.53956300
C	-1.50509900	1.17696500	0.74152400	C	-1.51604000	1.21136800	0.76206700
C	-0.58611500	0.08907800	0.55989200	C	-0.57484600	0.14989200	0.60558800
C	-0.99240300	-1.22931600	0.52325300	C	-0.99639400	-1.17513900	0.61630900
C	-2.31715200	-1.68551000	0.36727800	C	-2.31245900	-1.64897300	0.43300000
C	-3.34578600	-0.79552800	0.24596300	C	-3.37332700	-0.78874300	0.25425500
C	1.18189200	-1.29333100	0.24929400	C	1.17916900	-1.25724900	0.31978500
C	0.83899100	0.06779400	0.32934000	C	0.84603100	0.10778500	0.34904500
C	2.47896800	-1.74052000	0.07991700	C	2.47192200	-1.71875300	0.15533200
C	1.85077200	1.02590600	0.23396000	C	1.86164400	1.05498900	0.20594500
C	3.47645100	-0.77109900	-0.02710500	C	3.47381300	-0.76052200	-0.00185100
C	3.16265500	0.60114400	0.04694600	C	3.16922600	0.61532500	0.02050200
O	0.07558300	-2.08831500	0.36746900	O	0.07090900	-2.04184700	0.48261400
H	1.63472700	2.08370600	0.30355700	H	1.65146400	2.11573700	0.23867800
H	-1.22265700	2.14223300	0.32079500	H	-1.35687600	2.16749300	0.27071400
H	-2.49276800	-2.74334400	0.22506100	H	-2.45091000	-2.71037500	0.27488600
H	2.71286400	-2.79471900	0.02567500	H	2.69922900	-2.77567100	0.14113200
C	-2.61122700	1.17066200	1.68045800	C	-2.59938400	1.06997500	1.71012400
H	-2.96786900	1.98304100	2.29760600	H	-2.58643500	0.59617600	2.68534500
Br	4.50954200	1.94987200	-0.09191400	Br	4.52184300	1.94907300	-0.18643500
Br	5.26489800	-1.38555300	-0.27642200	Br	5.25547400	-1.39609800	-0.24591000
Br	-5.04823000	-1.49789700	-0.28462500	Br	-4.99379000	-1.53037100	-0.44675200
Br	-4.40314600	1.86375800	-0.47068000	Br	-4.45606400	1.89431600	-0.35775000
		TS4-Br				TS8-Br	

C	-3.11397900	0.64690700	0.11215500	C	-2.91413800	0.65588600	0.23107800
C	-1.83868300	1.22933700	0.50532400	C	-1.65314400	1.07394900	0.52932800
C	-0.60694000	0.06990600	0.86737300	C	-0.68736400	0.14398100	1.07840700
C	-1.06326300	-1.28902200	0.60339800	C	-1.13054300	-1.52871100	0.95783400
C	-2.35204200	-1.67624500	0.44915100	C	-2.38680400	-1.77495000	0.30195900
C	-3.37820900	-0.68744100	0.24823500	C	-3.27427400	-0.75512500	0.11603500
C	1.12221400	-1.29924100	0.24417900	C	1.06032800	-1.33056800	0.42199600
C	0.82754100	0.03978300	0.51623100	C	0.73576200	0.01222100	0.66098600
C	2.39457500	-1.73601500	-0.06940100	C	2.34021600	-1.72743600	0.07674800
C	1.84299700	0.98374800	0.49305200	C	1.71441900	0.98336600	0.50894700
C	3.40969800	-0.77528500	-0.11079200	C	3.31969200	-0.74181400	-0.06523100
C	3.13870400	0.57346400	0.16799300	C	3.00979700	0.60834100	0.14110700
O	0.01611900	-2.11160000	0.33586300	O	0.01002000	-2.21045900	0.50096200
H	1.64939300	2.02423400	0.71888500	H	1.49373300	2.02783400	0.68632400
H	-1.49606000	2.11136300	-0.02956400	H	-1.35189900	2.08851500	0.29740600
H	-2.59339400	-2.71808600	0.29028500	H	-2.60451100	-2.77287400	-0.05838800
H	2.59976600	-2.77676400	-0.27825500	H	2.56894300	-2.76984500	-0.09671500
C	-1.28622100	0.93815500	1.81397300	C	-1.06523500	-0.74786100	2.17157000
H	-1.77303000	0.71138200	2.75374500	H	-1.89194000	-0.58491700	2.85114900
Br	4.50044200	1.91142800	0.13089800	Br	4.31019900	1.99390500	-0.04308400
Br	5.16103700	-1.38194100	-0.55847800	Br	5.07001900	-1.31561100	-0.55992200
Br	-5.12390800	-1.40116000	-0.07389100	Br	-5.00453000	-1.24397100	-0.54120700
Br	-4.34025700	1.88402700	-0.67530600	Br	-4.16730900	2.00760100	-0.29784600
	TS11-Br				TS13-Br		
C	-2.97946400	0.60963500	0.26280300	C	-2.94118400	0.66567800	0.30118000
C	-1.60396400	0.93947500	0.52499400	C	-1.62055300	0.95452000	0.46106600
C	-0.66451900	-0.03075300	0.67351400	C	-0.63150500	-0.06514500	0.56017500
C	-1.02644100	-1.45163900	0.82188000	C	-0.96818300	-1.40196700	0.56172400
C	-2.55959700	-1.83641200	0.39066700	C	-2.26764500	-1.97144800	0.68868800
C	-3.40019200	-0.67096600	0.06512600	C	-3.52155700	-0.66351600	0.45075500
C	1.15692200	-1.36948500	0.33557700	C	1.19826400	-1.36690900	0.22442400
C	0.77533500	-0.02751000	0.48903300	C	0.80608400	-0.02804500	0.37485100
C	2.45806500	-1.74405000	0.05142900	C	2.50581200	-1.76081500	0.01377900
C	1.73334500	0.97470400	0.36006000	C	1.77803700	0.96973000	0.29994400
C	3.41242300	-0.72971700	-0.06161200	C	3.46718800	-0.75186300	-0.05471400
C	3.05513400	0.62085200	0.09386600	C	3.10435400	0.60185600	0.08698400
O	0.11700300	-2.24267400	0.48179300	O	0.11836500	-2.20909100	0.31872700
H	1.46991800	2.01878600	0.46678400	H	1.52323100	2.01561500	0.40826800
H	-1.31505800	1.98007800	0.45593400	H	-1.30514800	1.98852700	0.40296200
H	-2.72875800	-2.73510900	-0.20112700	H	-2.41373100	-2.95151600	0.23514600
H	2.73027900	-2.78322500	-0.07008500	H	2.77572600	-2.80194400	-0.09639900
C	-1.99660300	-1.98389500	1.72436300	C	-3.29380800	-1.48681700	1.59704000
H	-2.21177900	-2.26285300	2.74116300	H	-4.01395900	-2.07989500	2.14203800
Br	4.33463600	2.03164000	-0.05055200	Br	4.39942700	2.00417700	-0.00315400

Br	5.20629500	-1.26147300	-0.42664800	Br	5.27443100	-1.28875700	-0.34791800
Br	-5.09170100	-1.11033700	-0.69853200	Br	-5.06792900	-1.14206600	-0.65833100
Br	-4.13618100	2.10937700	-0.01390200	Br	-4.12606800	2.12180000	-0.10594700
TS14-Br							
C	-2.94721700	0.67048000	0.29965000				
C	-1.61035800	0.90984800	0.50055700				
C	-0.64135400	-0.12747700	0.60343400				
C	-0.97056000	-1.47539000	0.53426000				
C	-2.27429500	-2.01374200	0.64874300				
C	-3.54733000	-0.62506400	0.47579700				
C	1.19292500	-1.40240300	0.17458400				
C	0.79667800	-0.07731800	0.40993200				
C	2.49979600	-1.77530600	-0.07494200				
C	1.76291900	0.92816300	0.38321600				
C	3.45586200	-0.75900300	-0.09374600				
C	3.08871300	0.58159600	0.13343100				
O	0.11978700	-2.25654700	0.22841800				
H	1.50431000	1.96424800	0.55743700				
H	-1.25860600	1.93135900	0.42617900				
H	-2.52979500	-2.93343100	0.12903600				
H	2.77294100	-2.80636500	-0.25171100				
C	-3.19623300	-1.43048300	1.60527700				
H	-3.03523300	-1.12335000	2.63184800				
Br	4.37594700	1.99377800	0.11388800				
Br	5.26161000	-1.26759000	-0.44047700				
Br	-5.14597300	-1.13786500	-0.51158300				
Br	-4.03641800	2.14300600	-0.27386500				