

Density Functional Theory Study of Addition Reactions of Carbon-Centered Radicals to Alkenes

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SUPPORTING INFORMATION

Table S1: Calculated pre-exponential factors (logA, mol/l/s) for the addition of carbon-centered radicals to monosubstituted and 1,1-disubstituted alkenes CH₂=CXY at room temperature (300 K).

Radical	nonpolar-nucleophilic		nucleophilic		ambiphilic-electrophilic	
	Me	Bn	tBu	POH	PEst PCN	MEst MCN
H,Me	9.69		7.89		/	8.87
					7.75	/
Me,Me	9.72		7.84		/	8.98
					7.57	/
Me,Ome	9.75		8.01		/	8.65
					7.99	/
H,Cl						
Me,Cl	9.75		7.92		/	9.06
					7.87	/
Cl,Cl	9.79		7.04	8.87	/	
				/	7.99	
H,CO ₂ Me		8.77	7.75			9.14
						/
Me,CO ₂ Me			8.25			9.22
						/
H,CN			7.93			9.03
						/
H,CHO	9.70		8.04		/	9.14
					7.61	/
Me,CN	10.08		8.25		/	9.41
					8.04	/
H,Ph		8.56	7.76			8.87
						/
Me,Ph	9.65		8.05		/	8.69
					7.87	/

Table S2: Correlation between determined and experimental activation energies (reported as R² values).

Basis Set	Me	Bn	tBu	POH	MOH	Pest	PCN	MEst	MCN	FAc
6-31g(d,p)	0.67	0.77	0.95	0.64	0.19	0.71	0.69	0.52	0.55	0.29
6-311+g(d,p)	0.81	0.74	0.92	0.77	0.66	0.46	0.40	0.57	0.43	0.87

Table S3: Correlation between d and experimental activation energies (reported as R² values).

Basis Set	Me	Bn	tBu	POH	MOH	Pest	PCN	MEst	MCN	FAc
6-311+g(d,p)	0.94	0.67	0.76	-	0.76	0.88	0.85	0.68	0.70	-

Table S4: parameters of the EPS relation determined applying enthalpy changes and activation energies calculated both at the medium and large level of theory.

B3LYP/6-31g(d,p)				B3LYP/6-311+g(d,p)			
	C	α	R ²		C	α	R ²
Me	0.3763	14.413	0.5748	Me	0.3629	13.896	0.7832
Bn	0.4883	13.855	0.8730	Bn	0.5097	14.036	0.8250
tBu	0.6851	17.433	0.9123	tBu	0.5352	13.507	0.7215
POH	0.4045	9.9555	0.5502	POH	0.7053	14.864	0.7768
MOH	0.1539	6.2942	0.1495	MOH	0.5101	15.898	0.6130
PEst	0.6460	14.798	0.7628	PEst	0.6925	14.830	0.6607
PCN	0.4971	13.784	0.9503	PCN	0.4624	13.279	0.8549
MEst	0.2165	8.0315	0.5811	MEst	0.2069	8.5807	0.5455
MCN	0.3727	12.086	0.9123	MCN	0.2280	9.6636	0.4692
FAc	0.2364	7.1087	0.6063	FAc	0.1183	5.7302	0.0908

Table S5. Distance d between carbon atoms in the transition state structure of the addition reactions. Structures are determined at the B3LYP/6-311+G(d,p) level of theory, distances are reported in angstrom..

Alkene		Nucleophilic			Ambiphilic-Electrophilic				Electroph.
X	Y	tBu	POH	MOH	PEst	PCN	MEst	MCN	FAc
H	Me	2.27	2.26	2.31	2.26	2.28	2.28	2.20	2.23
Me	Me	2.27	2.26	2.31	2.19	2.29	2.29	2.19	2.24
Me	OMe	2.30	2.29	2.34	2.21	2.31	2.31	2.22	-
H	Cl	2.31	2.31	2.36	2.21	2.30	2.30	2.21	2.26
Me	Cl	2.30	2.30	2.35	2.21	2.31	2.31	2.21	2.26
Cl	Cl	2.35	2.34	2.39	2.24	2.34	2.34	2.23	2.30
H	CO ₂ Me	2.38	-	2.43	2.25	2.35	2.35	2.22	2.29
Me	CO ₂ Me	2.38	2.43	2.47	-	2.36	2.36	2.25	2.31
H	CN	2.42	-	2.49	2.27	2.37	2.37	2.26	
H	CHO	2.49	-	2.43	2.27	2.41	2.41	2.26	2.34
Me	CN	2.40	-	2.44	2.27	2.37	2.37	2.26	2.33
H	Ph	2.40	2.41	2.45	2.29	2.40	2.40	2.29	2.37
Me	Ph	2.39	2.45	2.46	2.28	2.40	2.40	2.28	2.37

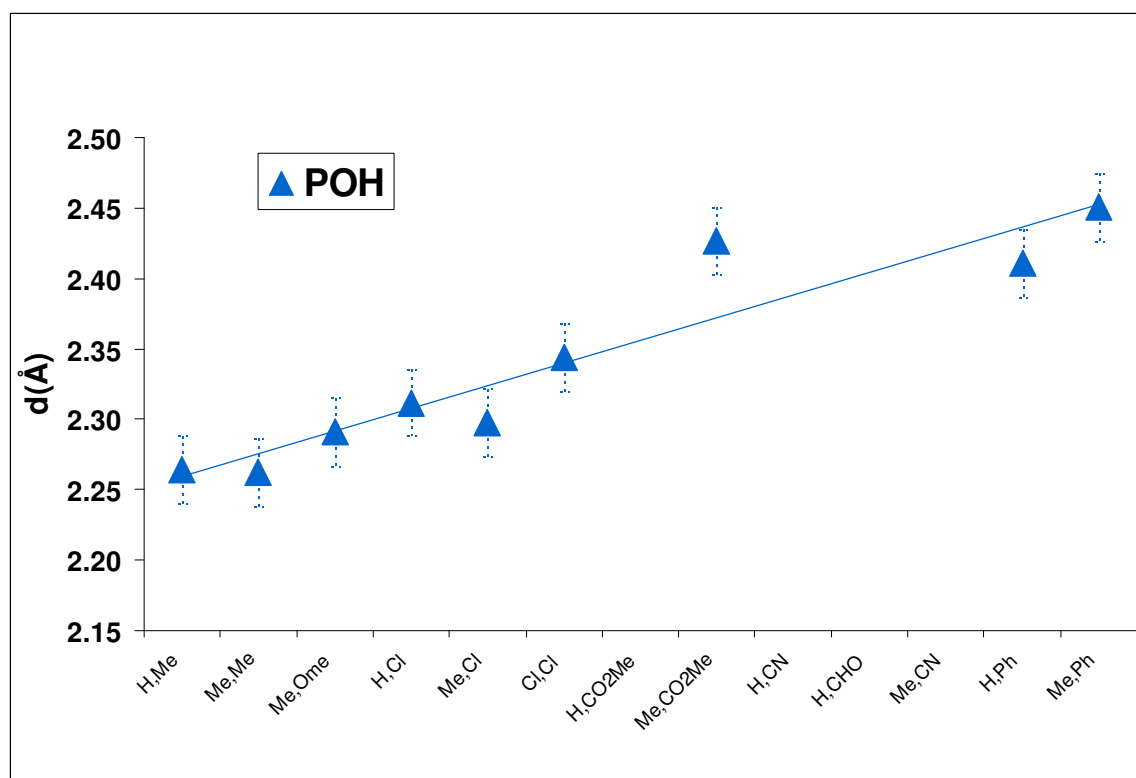
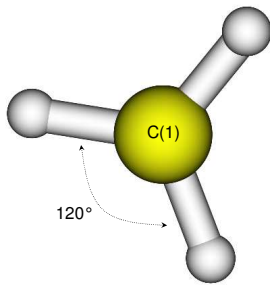
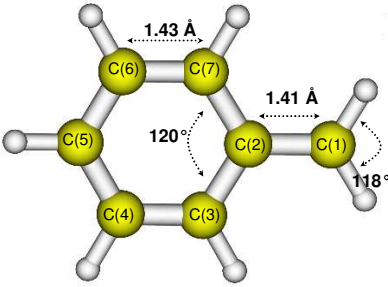
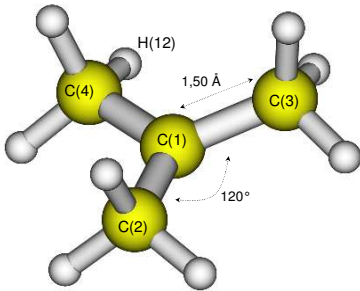
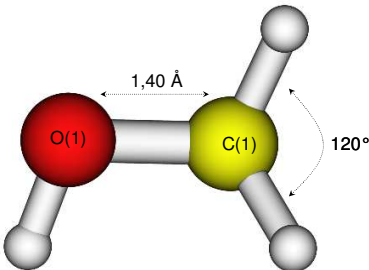
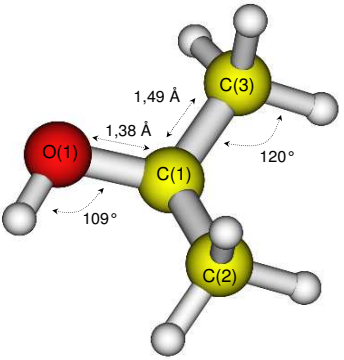
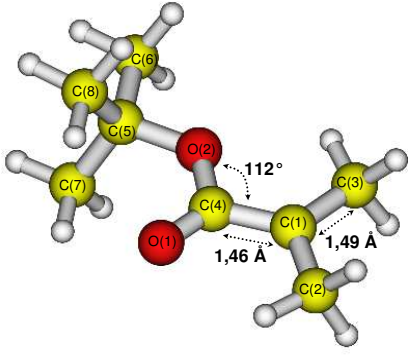


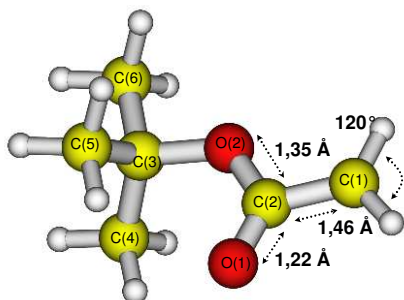
Figure S1: Distance d between carbon atoms in the transition state structure of the addition reactions between different unsaturated compounds and POH radical.

Table S4. Reactants geometries

Me	
	C,0,-0.0001555852,0.000440079,0.
	H,0,0.5105522023,0.1795100727,0.9373684643
	H,0,0.5105522023,0.1795100727,-0.9373684643
	H,0,-1.0201708933,-0.3616606198,0.
Bn	
	C,0,-1.1336023724,-1.2116551847,0.0001705513

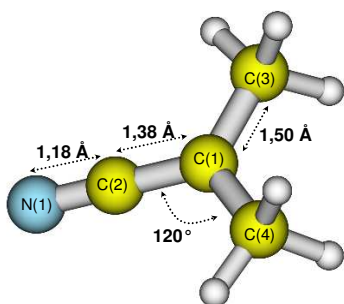
	C,0,0.2518201123,-1.2181152083,0.0008308719 C,0,0.9954325404,-0.0000429788,0.0004572628 C,0,0.2519257895,1.2180915739,-0.0005932869 C,0,-1.1334944341,1.2117505711,-0.0012237019 C,0,-1.8394775801,0.0000772378,-0.0008621998 H,0,-1.6762007249,-2.1528795934,0.0004537287 H,0,0.7932875046,-2.1603955637,0.0016018259 H,0,0.7934767829,2.1603238628,-0.0009076626 H,0,-1.6760134089,2.1530202952,-0.002018937 H,0,-2.925106049,0.0001267175,-0.0013623455 C,0,2.4014602447,-0.0000985729,0.0010940835 H,0,2.9630488273,-0.9278331711,0.0020492892 H,0,2.9631212657,0.9275928237,0.000942616
tBu 	C,0,-0.0479477717,0.1360473542,0. C,0,-1.3989279211,-0.5096307137,0. H,0,-1.9806959605,-0.2349134256,0.8879321928 H,0,-1.9806959604,-0.2349134256,-0.8879321929 H,0,-1.3334380974,-1.6135425739,0. C,0,0.7067460232,0.2342076506,-1.2894603915 H,0,1.4955555054,0.9943970795,-1.242245412 H,0,1.2059703627,-0.7166246273,-1.5532344704 H,0,0.0460400802,0.4794164356,-2.1295424293 C,0,0.7067460232,0.2342076505,1.2894603916 H,0,1.2059703626,-0.7166246273,1.5532344704 H,0,1.4955555053,0.9943970794,1.2422454121 H,0,0.0460400801,0.4794164356,2.1295424293
MOH 	C,0,0.1250346692,-0.6768797418,0.0432345425 H,0,0.704965576,-1.1134093253,-0.7608177542 H,0,0.2429228051,-1.045871217,1.0597161421 O,0,-0.1372660264,0.653062743,-0.1481625162 H,0,-0.5999681854,0.9960570493,0.6269944871
POH	C,0,-0.2211166454,0.0196656553,-0.0173130987

	O,0,0.0189750297,1.3784552668,-0.1286206233 H,0,-0.1468302445,1.7916985862,0.7291235399 C,0,0.0190423522,-0.606748511,1.3202497848 H,0,1.0920448093,-0.6491276635,1.5836385425 H,0,-0.4852550439,-0.0520737459,2.1238714284 H,0,-0.3612720038,-1.6323214069,1.3437719144 C,0,0.0799293608,-0.7095005397,-1.2836643491 H,0,-0.3456260176,-0.1805548216,-2.1424927976 H,0,1.1650838653,-0.8048753531,-1.4674167175 H,0,-0.3370760073,-1.7208873568,-1.2571649457
PEst	
	C,0,-1.444998 -2.626323 0.000000 C,0,-0.931656 -1.900367 -1.257405 H,0,-0.337201 -1.059702 -0.966188 H,0,-0.337220 -2.572912 -1.839839 H,0,-1.763874 -1.564088 -1.839839 C,0,-0.931656 -1.900367 1.257405 H,0,-0.337220 -2.572912 1.839839 H,0,-0.337201 -1.059702 0.966188 H,0,-1.763874 -1.564088 1.839839 C,0,-2.984998 -2.626304 0.000000 O,0,-3.639471 -3.664559 0.000000 O,0,-3.601743 -1.336139 0.000050 C,0,-5.023780 -1.486842 0.000044 C,0,-5.687268 -0.097100 0.000166 H,0,-5.385719 0.442018 0.873847 H,0,-5.385772 0.442145 -0.873456 H,0,-6.751310 -0.209864 0.000190 C,0,-5.457753 -2.262754 -1.257424 H,0,-6.009101 -1.613217 -1.904740 H,0,-4.591079 -2.625170 -1.769705 H,0,-6.074606 -3.088983 -0.971524 C,0,-5.457741 -2.262968 1.257386 H,0,-4.591056 -2.625332 1.769683 H,0,-6.009221 -1.613584 1.904742 H,0,-6.074463 -3.089242 0.971338
MEst	C,0,1.4133885898,-2.3749504964,-0.1238011406



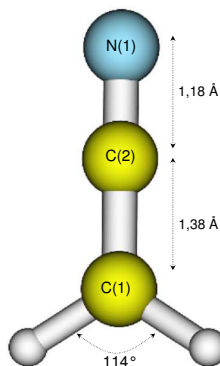
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H,0,0.6256413556,-3.1178055011,-0.1085670844
C,0,1.1140781522,-0.9563996974,-0.0735454735
O,0,1.9764435293,-0.0856919087,-0.0885193933
O,0,-0.2233056952,-0.7412933752,-0.0092556438
C,0,-0.7810021271,0.6198604096,0.0502789985
C,0,-0.3014238201,1.3277922461,1.322380654
H,0,-0.5440609783,0.7276326445,2.2049256147
H,0,0.7747016191,1.5003911045,1.2966883433
H,0,-0.810228997,2.2924898226,1.4180635656
C,0,-0.4121984743,1.3938388026,-1.2202900956
H,0,0.6623896136,1.5678753813,-1.2790488473
H,0,-0.7315003927,0.8394894788,-2.1083718468
H,0,-0.9257089231,2.3607907346,-1.221431684
C,0,-2.2882715876,0.3609121411,0.1091739263
H,0,-2.8316356094,1.309154634,0.1576393577
H,0,-2.6205119021,-0.1844892021,-0.7786811148
H,0,-2.5433806537,-0.2308123611,0.992866554

PCN



C,0,0.0463027326,-0.3055402777,0.0000612928
C,0,-0.1612688616,1.0705990764,0.0000621409
N,0,-0.3392456554,2.2337030179,-0.0001709067
C,0,0.1595304597,-1.0532119822,-1.2963969591
H,0,0.0566855987,-0.3954491123,-2.1612284238
H,0,1.1293643847,-1.5647763668,-1.3642256496
H,0,-0.6113628379,-1.8331897067,-1.3608045107
C,0,0.1596096155,-1.0533031067,1.296451722
H,0,1.1294518917,-1.5648637164,1.3641948503
H,0,0.0568064776,-0.3956087957,2.1613419403
H,0,-0.6112696046,-1.8332956866,1.3608489616

MCN



C,0,1.1958320092,-0.0000566624,0.0045673439
H,0,1.7450084008,0.0115154161,-0.929247853
H,0,1.7373387179,-0.011684152,0.9428493547
C,0,-0.1859807646,0.000012187,-0.0009826483
N,0,-1.3630649409,0.0000622269,-0.0050156679

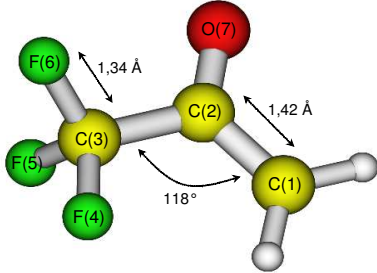
FAc	C,0,-0.5459979882,0.1414546169,0.1230940339 C,0,0.9324847354,-0.1323181408,-0.2334746133 C,0,1.5028696541,-1.3751607231,0.153920891 H,0,0.9439260515,-2.116696909,0.7108643398 H,0,2.5308297369,-1.5739202287,-0.1262704886 F,0,-1.3235528784,-0.0522916016,-0.9593470488 F,0,-0.7084942302,1.4034632684,0.5377066328 F,0,-0.9874832435,-0.6838700961,1.0996070404 O,0,1.5456098714,0.7351310603,-0.8684419174
	

Table S5. Monomers geometries

X=H, Y=Me	C,0,0.5199385751,-0.1741995957,-1.1802770926 C,0,0.4322836799,0.164193722,0.1058416268 H,0,1.4398811064,-0.0483469856,-1.7432480023 H,0,-0.3282993225,-0.5907042079,-1.7188218479 H,0,1.3109716441,0.5782568103,0.6016256017 C,0,-0.7969093306,0.0245563758,0.9564045213 H,0,-1.1133712653,0.9954984358,1.3582331499 H,0,-1.6320780798,-0.397455664,0.389430994 H,0,-0.6089816289,-0.6245514018,1.8209657714
X=Me, Y=Me	C,0,-0.0013933887,-0.0003680256,-1.4559536735 C,0,0.0045754003,-0.0000637951,-0.1199032851 H,0,0.9208382909,-0.0003074873,-2.0298790998 H,0,-0.9280718783,-0.0006894562,-2.0242360468 C,0,-1.2843794611,-0.0000129955,0.684411526 H,0,-1.8938979612,0.8826096357,0.4620539375 H,0,-1.8956538443,-0.8807365106,0.4594016389 H,0,-1.089414095,-0.0017962065,1.7607419157 C,0,1.2867360211,0.0003618624,0.6728791246 H,0,1.3422726734,0.8794067014,1.3285299775 H,0,1.3426621294,-0.8784464991,1.3288117179 H,0,2.1680332552,0.0004575453,0.0259738072
X=Me, Y=OMe	C,0,-1.8473382434,-0.0287826118,0.0466818351 C,0,-0.5262690214,-0.1882435158,-0.0774931162 H,0,-2.284230677,0.9623175268,0.0809513029 H,0,-2.5074231551,-0.886273125,0.0868755267 C,0,0.1594467125,-1.5270563904,-0.1359581464 H,0,0.8431990705,-1.6817152522,0.7067137672 H,0,-0.5821132384,-2.3274685321,-0.1143231344 H,0,0.7485010439,-1.6266546899,-1.0556288696 O,0,0.2490950995,0.9388476623,-0.2406415226 C,0,1.5582705281,0.9374463048,0.311131251 H,0,1.5432068699,0.7791400284,1.3978849579

	H,0,2.2086344696,0.1834569556,-0.14925416 H,0,1.9728049659,1.9262330697,0.1057418487
X=H, Y=Cl	C,0,-1.4953996956,-0.7353791383,-0.0000230595 C,0,-0.171854996,-0.7464386872,-0.00001524 H,0,-2.0700056423,0.1820798426,-0.0000083503 H,0,-2.033605943,-1.6759365938,-0.0000452904 H,0,0.4315215307,-1.6438604225,-0.0000298257 Cl,0,0.8044481297,0.7075661251,0.0000184273
X=Me, Y=Cl	C,0,-1.5946251563,-0.2470130958,-0.4187322711 C,0,-0.2966580993,-0.3340088875,-0.1412800565 H,0,-2.1445990365,0.6826373138,-0.340022008 H,0,-2.1342525804,-1.1333843538,-0.7368053594 C,0,0.5565643401,-1.5625581258,-0.2164078878 H,0,0.9979219512,-1.7918238755,0.7592471716 H,0,-0.0428299711,-2.4172689304,-0.540801521 H,0,1.3815313025,-1.4224225512,-0.9228369504 Cl,0,0.5853259899,1.1143378266,0.3788082329
X=Cl, Y=Cl	C,0,0.000021928,-0.0000089903,-1.7537171371 C,0,0.0000057557,-0.0000017811,-0.4250401594 H,0,0.9331464597,0.0000072593,-2.3032770131 H,0,-0.9330894342,-0.0000313458,-2.3032993542 Cl,0,1.4663270385,0.0000327687,0.5199925196 Cl,0,-1.4663401636,-0.0000275502,0.5199557243
X=H, Y=CO₂Me	C,0,-2.1354344329,1.2818486293,0.0000158824 C,0,-0.8025309405,1.2287904766,-0.000017163 H,0,-2.6692720291,2.2263189401,-0.0000423379 H,0,-2.718249654,0.3657179965,0.0001028794 H,0,-0.1838297182,2.120621252,-0.0001028536 C,0,-0.0974084574,-0.0779725818,0.0000653944 O,0,-0.6253060503,-1.1718812103,0.000094138 O,0,1.2446296205,0.105343846,-0.0000542865 C,0,2.0245615592,-1.0999706566,-0.0000728469 H,0,1.808323897,-1.6991956823,0.8880664053 H,0,1.8077298682,-1.6995626293,-0.887815226 H,0,3.0655827036,-0.7777761682,-0.0004752808
X=Me, Y=CO₂Me	C,0,-2.1591916376,0.8253378306,0.0000600361 C,0,-0.8214950868,0.8608255038,-0.0000040135 C,0,-0.1069484263,-0.4561818474,-0.0000958102 O,0,1.2382664702,-0.2904969591,-0.0001232436 C,0,2.00211545,-1.5061008617,-0.0000341942 O,0,-0.6370157811,-1.5494360577,0.000135987 H,0,-2.7497827097,1.7361127868,0.0001448836 H,0,-2.6830051067,-0.1242027427,0.0000383941 C,0,-0.0128166215,2.1316781388,0.0000183975 H,0,1.7769651862,-2.1020379197,0.8878965148 H,0,1.7765456075,-2.1024456723,-0.8875803841

	H,0,3.0474919705,-1.1979613923,-0.0003406873 H,0,-0.6685620763,3.0058673978,0.0000908502 H,0,0.6402198338,2.1853466068,0.8772189211 H,0,0.6401397148,2.185432486,-0.8772369339
X=H, Y=CN	C,0,-0.726400987,-0.2679789347,-0.0000683682 C,0,0.7017284238,-0.3584121235,0.0000160881 C,0,-1.3822993917,0.8983067337,-0.0000168281 N,0,1.8611576351,-0.455342163,0.0000833119 H,0,-0.8592078973,1.8485614493,0.0000932254 H,0,-2.4666062794,0.9220461237,-0.0000837713 H,0,-1.2604575395,-1.2147064852,-0.0001779883
X=H, Y=CHO	C,0,-0.8959569017,-0.0000644625,-1.2527350337 C,0,-0.8951085083,-0.0000181817,0.0846704117 H,0,0.0457378282,-0.0000768428,-1.7943383504 H,0,-1.8142905941,-0.0000866865,-1.830839431 H,0,-1.8211638285,0.000000903,0.6554323502 C,0,0.3722295036,0.0000254487,0.8576865413 O,0,1.4816705375,0.0000632404,0.3586774087 H,0,0.249367733,-0.0000001233,1.9625946458
X=Me, Y=CN	C,0,-1.6174447682,-0.2657350058,-0.0001415305 C,0,-0.2764393125,-0.2984503974,-0.00005356 H,0,-2.1659341834,0.6692402729,-0.0000996433 H,0,-2.1955518802,-1.1848943216,-0.0002594942 C,0,0.540942095,-1.5801182954,-0.0000700603 H,0,0.3140481414,-2.1821769998,0.8850604705 H,0,0.3132405688,-2.1826676852,-0.8846564756 H,0,1.6116016612,-1.3695706749,-0.0006080548 C,0,0.454908064,0.9393892942,0.0000986757 N,0,1.0729713175,1.9256508335,0.0002231497
X=H, Y=Ph	C,0,-0.3545356404,-0.0002346159,-1.0333637491 C,0,-0.4187644623,-0.0000030812,0.3721895588 C,0,0.791306077,0.0002732299,1.0866601658 C,0,2.0200562698,0.0003263078,0.4282025853 C,0,2.0651716199,0.0000978477,-0.9656700582 C,0,0.8707045059,-0.0001865033,-1.6923357068 C,0,-1.6862478484,-0.0000332046,1.121131295 C,0,-2.9293019663,-0.000213337,0.6251169024 H,0,-3.1391999253,-0.0003587662,-0.4403181695 H,0,-3.7913282881,-0.0002189649,1.2837663645 H,0,0.7626129003,0.0004516691,2.1735038362 H,0,2.9409604436,0.0005495046,1.0042199804 H,0,3.0198790661,0.0001377409,-1.4832263439 H,0,0.896294226,-0.0003659604,-2.7783610331 H,0,-1.2707802999,-0.0004659521,-1.615623001 H,0,-1.5687694543,0.000110869,2.2044524074

X=Me, Y=Ph	C,0,-1.4118235626,-0.265915858,-2.2646650808 C,0,-1.4067526487,0.0105045789,-0.9516300323 H,0,-0.5135595313,-0.5540455783,-2.800424489 H,0,-2.3304773642,-0.231075442,-2.8421539113 C,0,-0.1516567919,-0.0041758332,-0.1508575784 C,0,-0.1693415146,-0.297379692,1.223807172 C,0,1.0081633921,-0.3282349399,1.9707955901 C,0,2.2336446296,-0.053879222,1.364701996 C,0,2.2685219231,0.2570611592,0.0035695598 C,0,1.0924039798,0.2860911913,-0.740913 H,0,-1.1102081005,-0.518674757,1.7167574317 H,0,0.9653034146,-0.566968204,3.0297262584 H,0,3.1502442526,-0.0718289616,1.946882426 H,0,3.2141407289,0.4908412266,-0.4774305517 H,0,1.1312915343,0.5630184644,-1.789552832 C,0,-2.6966579171,0.3355346671,-0.2321124169 H,0,-3.5222729096,0.4377011954,-0.9403905988 H,0,-2.9710187393,-0.4525181759,0.4796989872 H,0,-2.6124522247,1.2659139245,0.3407100221
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Table S6. Transition states geometries

Me + X=H, Y=Me	C,0,2.1177911102,-0.5582467174,0.0920873556 C,0,0.2918773679,0.881515596,-0.3117569224 H,0,2.8650766479,-0.0723636255,-0.5266607166 H,0,2.2217397252,-0.4508971331,1.1654823623 H,0,1.7139945917,-1.4969039679,-0.2692319631 H,0,0.9006583296,1.6985538082,0.0602125528 H,0,0.3975716475,0.6488840326,-1.3675797672 C,0,-0.7947280631,0.4551465151,0.3819669923 H,0,-0.9383904188,0.8107847706,1.4019763353 C,0,-1.7826269854,-0.5550507555,-0.11763446 H,0,-1.5788504393,-0.8377122187,-1.155193932 H,0,-1.7661272601,-1.4706212441,0.4899698814 H,0,-2.8095534006,-0.1699122516,-0.0669525462
Me + X=Me, Y=Me	C,0,-0.5456639822,-0.0001778671,0.9563783435 C,0,0.6068150151,-0.0000031433,0.2315200232 H,0,-0.9281654153,-0.9212373611,1.3842778524 H,0,-0.9282548356,0.9207093412,1.3845697892 C,0,1.250614352,1.2782093201,-0.2333086516 H,0,2.3016882079,1.3310664854,0.0816283347 H,0,1.25564791,1.346220059,-1.3307015901 H,0,0.7353238227,2.1606201582,0.1559230336 C,0,1.250894444,-1.2780126588,-0.2334797043

	H,0,1.2559358904,-1.3458821541,-1.3308816313 H,0,2.3019826129,-1.3306739777,0.0814428897 H,0,0.7358048644,-2.160588261,0.1556435181 C,0,-2.4050248149,-0.0000403355,-0.5065308314 H,0,-2.2357699099,0.923507695,-1.048122175 H,0,-2.2356776975,-0.9233926753,-1.0484269227 H,0,-3.2043255337,-0.0002012021,0.227171825
Me + X=Me, Y=OMe	C,0,-2.7428376586,-0.5222333736,-0.6095640639 C,0,-1.0560140741,0.0961243699,0.9672755134 H,0,-3.5668616311,-0.7241767105,0.0666730764 H,0,-2.8140881956,0.3730506362,-1.2170175985 H,0,-2.2419322846,-1.3768172765,-1.0485532093 H,0,-1.6497098881,0.9525600734,1.2575993527 H,0,-1.2420624293,-0.8433088443,1.471954777 C,0,0.1193932444,0.284106569,0.3118241206 C,0,0.5444047477,1.5936720052,-0.2878116008 H,0,-0.186685979,2.3668195469,-0.0442081684 H,0,1.5210966422,1.9300477555,0.08046916 H,0,0.6170304486,1.5287444018,-1.3818787386 O,0,0.864451854,-0.8407518986,0.037314065 C,0,2.2598403681,-0.6923125735,-0.1778056868 H,0,2.6468657174,-1.6980610367,-0.3521033226 H,0,2.4866693541,-0.0729344366,-1.0542216394 H,0,2.7653436487,-0.2660509027,0.699264096
Me + X=H, Y=Cl	C,0,2.4469241323,-0.7290962577,0.1183236682 C,0,0.7829457841,0.9229646258,-0.3748540219 C,0,-0.3090569717,0.7210934309,0.3912994438 H,0,3.2093575633,-0.4226037691,-0.5897007954 H,0,2.6229356324,-0.5163179817,1.1659970353 H,0,1.8647996107,-1.6109648302,-0.1200130753 H,0,1.486631358,1.6928141601,-0.0783232218 H,0,0.824155948,0.5740465814,-1.3992837385 Cl,0,-1.5931054016,-0.3735452246,-0.068567726 H,0,-0.4499659533,1.1435238642,1.3783605974
Me + X=Me, Y=Cl	C,0,0.8551306205,0.1424011616,0.9722591813 C,0,-0.2770322224,0.4092068915,0.2816189348 H,0,1.4658437371,0.972964803,1.3088248556 H,0,1.0054582987,-0.8142403454,1.4551196758 C,0,-0.6737599748,1.7262309835,-0.3043400206 H,0,-0.7087267236,1.6801952092,-1.3995024699

	H,0,-1.6698398647,2.0278692699,0.0383398442 H,0,0.043798137,2.4980458106,-0.0122790254 C,0,2.6056119484,-0.4704533479,-0.5435104671 H,0,2.12182714,-1.3204452641,-1.0092529078 H,0,2.6889573897,0.4376833007,-1.128967309 H,0,3.3911676717,-0.6728097064,0.1765066327 Cl,0,-1.376364001,-0.9207986594,-0.1097032392
Me + X=Cl, Y=Cl	C,0,0.9923917595,0.0000001262,1.0066152137 C,0,-0.1908222289,0.0000000019,0.3601796888 H,0,1.3912873243,0.9299174678,1.3900483694 H,0,1.3912874715,-0.9299171158,1.3900484574 C,0,2.8102722564,0.0000001932,-0.619475769 H,0,2.5684790576,-0.9273059075,-1.1242951982 H,0,2.5684789107,0.9273062078,-1.124295286 H,0,3.6487144205,0.0000002921,0.068071774 Cl,0,-0.9776262927,-1.4687206185,-0.149514428 Cl,0,-0.9776265253,1.4687204495,-0.1495145671
Me + X=H, Y=CO₂Me	C,0,2.8101656783,-0.2859511499,-0.3269378292 O,0,1.640808585,0.5354570311,-0.4476232161 C,0,0.5471217368,0.0805928638,0.2168017805 C,0,-0.5974912779,0.9901386972,0.0352405805 C,0,-1.7762132025,0.7373246742,0.6489757746 C,0,-3.064539781,-0.8113728327,-0.7766251395 O,0,0.5427475542,-0.949973932,0.8664677266 H,0,-2.6026169638,1.4357656907,0.5880570304 H,0,-1.8387744386,-0.0586973958,1.3822099716 H,0,3.1174102146,-0.3714929424,0.7186651941 H,0,2.6205210533,-1.2894032983,-0.7169744114 H,0,3.5833641549,0.2116287944,-0.9123700504 H,0,-3.9607118854,-0.8680973751,-0.1697109688 H,0,-3.0985715109,-0.2294152645,-1.6890374099 H,0,-2.3412865305,-1.6132722049,-0.7040013584 H,0,-0.4620421297,1.8347256879,-0.6323250831
Me + X=Me, Y=CO₂Me	C,0,-2.879988265,-0.3483939262,0.385467361 O,0,-1.6814007885,0.4244725923,0.2333615165 C,0,-0.6118247928,-0.2598880912,-0.2501756986 C,0,0.5857459081,0.6097240334,-0.377239031 C,0,1.7045809891,0.0427770861,-0.8941811534 C,0,2.9368084404,-1.0449074821,0.9607730516 O,0,-0.6626574871,-1.4441783459,-0.5319232782

	C,0,0.5226715899,2.0324310898,0.1092584215 H,0,2.5900385517,0.6368193629,-1.0911375314 H,0,1.6594363377,-0.955353341,-1.3116737639 H,0,-3.2028958943,-0.7548456952,-0.5764192287 H,0,-2.7194405884,-1.1788794963,1.0777432119 H,0,-3.6274908185,0.3398574868,0.7802011452 H,0,1.4776410128,2.5396100608,-0.0513771092 H,0,-0.2605354482,2.5951331038,-0.4097883804 H,0,0.2806563037,2.0804985239,1.1770976382 H,0,3.7950176068,-1.3826220281,0.3917290424 H,0,3.061940577,-0.1968310844,1.6223444627 H,0,2.1501353454,-1.7561971233,1.1763569001
Me + X=H, Y=CN	C,0,-2.3678306881,-0.8812708444,0.136399424 C,0,-0.721202942,0.8958405478,-0.4373681217 C,0,0.3560713373,0.7864814114,0.3800300208 C,0,1.4741256549,-0.0394349813,0.0748658522 N,0,2.3970264074,-0.7112555694,-0.1611699898 H,0,-1.5089466381,1.6030444812,-0.2075754432 H,0,-0.719966972,0.4574489101,-1.42808205 H,0,-1.7137258541,-1.7265421146,-0.0363736341 H,0,-2.5661256685,-0.5901054786,1.1603583749 H,0,-3.106667952,-0.6385299072,-0.6186075625 H,0,0.3892680607,1.3037762942,1.3349071912
Me + X=H, Y=CHO	C,0,0.854683206,0.9705503107,0.2194401443 C,0,-0.3032806184,0.6058471832,-0.384569891 H,0,1.5848989193,1.5975838223,-0.2783839045 H,0,0.9890453756,0.8241858399,1.2876397952 C,0,2.5311962286,-0.8415165549,-0.0931395928 H,0,1.9858795295,-1.6358933453,0.4004408161 H,0,2.5555562607,-0.8368088951,-1.175511036 H,0,3.3452979807,-0.3666565101,0.4420579342 H,0,-0.49427957,0.8158457269,-1.4338447463 C,0,-1.3479263132,-0.1163411244,0.3419119383 O,0,-2.4082216694,-0.4731196712,-0.1443612087 H,0,-1.1086601587,-0.3245381575,1.4106352184
Me + X=Me, Y=CN	C,0,0.7834464754,0.0739643077,0.9862560089 C,0,-0.3224749207,0.4152598348,0.2729607625 H,0,1.5031426956,0.8331698901,1.2704976378 H,0,0.8609069618,-0.8903549705,1.4728968314 C,0,2.5227919884,-0.759842857,-0.5786133296

	H,0,1.9497569904,-1.5774875143,-0.9973523848 H,0,2.6501663124,0.1332482508,-1.1778762866 H,0,3.279281279,-0.9900937447,0.1626259888 C,0,-1.3241234238,-0.5744030601,0.0160114098 N,0,-2.1561405118,-1.3593519308,-0.2076110665 C,0,-0.5469601788,1.7801867021,-0.3314093538 H,0,-1.4943823401,2.2108794018,0.010246424 H,0,0.2625996501,2.4594730572,-0.0539135423 H,0,-0.5945676094,1.7256395801,-1.4250801895
Me + X=H, Y=Ph	C,0,-2.7147636253,0.5471286264,0.2056147937 C,0,-1.697103728,1.4129053917,-0.2068978179 C,0,-0.4067609857,0.9370000577,-0.4145816357 C,0,-0.0949798594,-0.4239561904,-0.2168991824 C,0,-1.1322984522,-1.2790118975,0.2038213638 C,0,-2.4244914971,-0.8026956148,0.4104662809 H,0,-3.2055630915,-1.4853023682,0.7330614967 H,0,-0.9135958712,-2.3315361626,0.3660783322 H,0,-3.7207683374,0.922736863,0.3671109781 H,0,-1.9122975975,2.4660459761,-0.3649290112 H,0,0.3697920271,1.6274810252,-0.7286754338 C,0,1.2420032082,-0.9773518579,-0.4250415833 C,0,2.3418754606,-0.3200007761,-0.8721520551 C,0,3.5098911319,0.6941071197,1.0723246599 H,0,2.2912022834,0.6885057903,-1.2671468441 H,0,3.2594745572,-0.8614676217,-1.0693551628 H,0,2.6797132272,1.2844847397,1.4390141585 H,0,3.7586758145,-0.2147273414,1.605645276 H,0,4.3015726822,1.2015561456,0.5331241723 H,0,1.351564388,-2.0265261986,-0.1538569053
Me + X=Me, Y=Ph	C,0,-2.1146136686,-0.1903012364,-0.8982474917 C,0,-1.1840228392,0.6381311266,-0.3489167189 H,0,-3.1196260141,0.1680060236,-1.0892084919 H,0,-1.8419660549,-1.1172412196,-1.3875793725 C,0,-3.117777164,-1.5779209353,0.8969288333 H,0,-2.2038415208,-1.9877040142,1.3082892689 H,0,-3.6123015371,-0.7910597384,1.4528087367 C,0,-1.6018762775,2.0087131878,0.1312672328 H,0,-1.3202411108,2.1761528345,1.1777654753 H,0,-1.1285744885,2.8059618966,-0.4559044292 H,0,-2.6834284074,2.1376791086,0.0449392328 C,0,0.227832242,0.2365298645,-0.1745713812 C,0,1.2238077668,1.191685706,0.1107387381

	C,0,2.5600691692,0.824988835,0.2636311308 C,0,2.9428606557,-0.5107039903,0.1468185527 C,0,1.9691316226,-1.4766322786,-0.1210818392 C,0,0.6363110574,-1.1104470003,-0.2756005848 H,0,0.9559903726,2.2384374455,0.2037591866 H,0,3.303467889,1.5883325047,0.4756948842 H,0,3.9828274837,-0.798221962,0.2694825844 H,0,2.2493804687,-2.523342302,-0.2005931893 H,0,-0.1031832005,-1.8830586485,-0.456413864 H,0,-3.7288392662,-2.2182016018,0.2711611466
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Bn + X=H, Y=Me	C,0,1.9716779823,-0.3663933363,-0.7569450246 C,0,3.2873925122,-0.5130458764,-0.3922098847 H,0,1.6165374644,0.6008968922,-1.1031478227 H,0,1.4189588815,-1.2202370383,-1.1359662915 C,0,0.6961683601,-0.2530638237,1.0291604083 H,0,0.978347994,-1.2120624395,1.4512422426 H,0,1.1852922794,0.604295751,1.4802988845 C,0,-0.6542640102,-0.0914961056,0.5512918459 C,0,-1.470763595,-1.2122125438,0.2660087113 C,0,-2.7587001872,-1.055189347,-0.2328843173 C,0,-3.2754041924,0.2233023661,-0.4691327386 C,0,-2.4840695999,1.3447775302,-0.1983422354 C,0,-1.1955114313,1.1923786754,0.3004676942 H,0,-1.0789793022,-2.2095682844,0.4502102275 H,0,-3.3673762743,-1.9318929704,-0.4367809958 H,0,-4.2821754004,0.3440927678,-0.8574216694 H,0,-2.8782406372,2.341802895,-0.3750690536 H,0,-0.5892007139,2.0697951651,0.5120585678 C,0,4.2065948234,0.6236382875,-0.0681025416 H,0,5.1500560888,0.5473233999,-0.624775974 H,0,3.7514747005,1.5899494128,-0.3077066093 H,0,4.4802096056,0.6366168309,0.9971805841 H,0,3.6763713416,-1.517187341,-0.2259935952
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Bn + X=Me, Y=Me	C,0,1.5962022969,-0.0001476142,-0.7344872359 C,0,2.9208433811,0.000098426,-0.360860227 H,0,1.1407787138,0.9158533227,-1.0989667057 H,0,1.1410961596,-0.9163517225,-1.0988552842 C,0,0.3046554549,-0.0002936001,1.048431626 H,0,0.6894051193,-0.9148538531,1.4884431461 H,0,0.6894756763,0.9140992017,1.4887292871
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	C,0,-1.0511584942,-0.0001664937,0.5605325484 C,0,-1.7334666263,-1.2103094526,0.2863558937 C,0,-3.0258787351,-1.2077653725,-0.2252355303 C,0,-3.6823264312,0.0000929611,-0.4853034391 C,0,-3.0258144902,1.2078221794,-0.22479924 C,0,-1.7334022986,1.210112074,0.2867935404 H,0,-1.2331029313,-2.1541929816,0.4888337358 H,0,-3.5290110068,-2.1509212266,-0.4204236835 H,0,-4.6925578797,0.0001915423,-0.8832738557 H,0,-3.5288966587,2.151075729,-0.4196439493 H,0,-1.2329871041,2.1538952284,0.489611993 C,0,3.6600636699,1.278442871,-0.0789980952 H,0,3.9385393812,1.3577406082,0.9825959398 H,0,4.601187203,1.325369952,-0.6439781719 H,0,3.0667260285,2.1601552644,-0.3368823129 C,0,3.6604932508,-1.2779640604,-0.0788457435 H,0,4.6015882883,-1.324683738,-0.6438911207 H,0,3.9390752015,-1.3570013193,0.9827395896 H,0,3.0674179425,-2.1599075148,-0.3365431929
Bn + X=Me, Y=OMe	C,0,0.1489542213,0.155618137,1.0368476101 C,0,-1.1569518656,0.2268833253,-0.7680226299 H,0,-0.1597465304,1.10275962,1.4681700034 H,0,-0.3353069572,-0.7208044102,1.4545019424 H,0,-0.6869707308,1.1218446858,-1.1561562514 H,0,-0.7581388336,-0.7192239835,-1.113926108 C,0,-2.4729130306,0.2860466962,-0.3830371417 C,0,-3.2060900541,1.5640932675,-0.1000988828 H,0,-2.5893145096,2.4155916568,-0.3938299852 H,0,-4.1545470282,1.6360713415,-0.6460201893 H,0,-3.4421821237,1.6712330123,0.9682334643 O,0,-3.0550534374,-0.9105170874,-0.0359423393 C,0,-4.4709946671,-0.988467234,0.0385160441 H,0,-4.7016111416,-2.019202943,0.3135527594 H,0,-4.8882289376,-0.3192836636,0.8005183653 H,0,-4.9420991062,-0.7658288939,-0.9279482573 C,0,1.4990248909,0.0354771963,0.5576158751 C,0,2.0672439246,-1.2301777106,0.2676077803 C,0,3.3570888293,-1.342096261,-0.2375394484 C,0,4.1275980552,-0.1985624255,-0.4763026934 C,0,3.5857898194,1.0618843674,-0.2002513603 C,0,2.2964611762,1.1793944476,0.3047546879 H,0,1.4782863195,-2.1251324778,0.4531770908 H,0,3.769451125,-2.3260257548,-0.4447414835 H,0,5.1357536373,-0.28829208,-0.8694599034

	H,0,4.1770480747,1.956247473,-0.3783128933 H,0,1.8867664444,2.1636202805,0.5192411142
Bn + X=H, Y=Cl	C,0,0.2469296684,-0.3938000636,1.0315157811 C,0,1.5195479217,-0.5627095372,-0.782063916 H,0,0.4750435796,-1.3738806127,1.4373450976 H,0,0.8112762745,0.4267341447,1.4621938955 H,0,0.9586288606,-1.4110178373,-1.1609440925 H,0,1.193570641,0.415489545,-1.1163199383 C,0,2.8211013903,-0.7723823148,-0.4316556272 H,0,3.2575152296,-1.7461552564,-0.2479043382 C,0,-1.0878336308,-0.1415629437,0.557820471 C,0,-1.5359719833,1.1770742573,0.2998200742 C,0,-2.8129546952,1.4168477146,-0.1933475849 C,0,-3.6833828034,0.3518908853,-0.450530539 C,0,-3.2597179276,-0.9591611367,-0.2064570948 C,0,-1.9836539027,-1.2044043549,0.2863705318 H,0,-0.8669741147,2.0098544486,0.5016018507 H,0,-3.1364730371,2.4376226092,-0.3765666661 H,0,-4.6809204324,0.5415566094,-0.8349394687 H,0,-3.9315105566,-1.7908018563,-0.3996724975 H,0,-1.6632848125,-2.2255568501,0.4778153329 Cl,0,3.8963967143,0.5438470599,-0.0242024561
Bn + X=Me, Y=Cl	C,0,1.2452399514,0.2538225544,-0.7531531731 C,0,2.5581488513,0.3654045313,-0.3867745169 H,0,0.7491632758,1.1423016515,-1.1307678742 H,0,0.85371013,-0.6948046409,-1.0990244537 C,0,-0.0518560953,0.1693061371,1.0501190395 H,0,0.426520083,-0.7102733963,1.4681133545 H,0,0.2626951635,1.1147324526,1.4803954132 C,0,-1.4001730363,0.0560044819,0.5614909466 C,0,-2.1877127569,1.2052302091,0.3063809104 C,0,-3.4763212224,1.0942546614,-0.2019850638 C,0,-4.0220920968,-0.1643275136,-0.4777672134 C,0,-3.2602612654,-1.3129859752,-0.2366098132 C,0,-1.9712237658,-1.2075353701,0.2719420234 H,0,-1.7726933101,2.1867452203,0.522095363 H,0,-4.0630349814,1.9906874855,-0.38260927 H,0,-5.0295363982,-0.2489776113,-0.87365455 H,0,-3.6781918133,-2.2940741162,-0.4443021209 H,0,-1.387211612,-2.1048516566,0.4607367803 Cl,0,3.4587284862,-1.1075014722,-0.0081577952 C,0,3.295004479,1.6328673335,-0.0987758396

	H,0,3.5439028912,1.7223412163,0.9665601979 H,0,4.2392566975,1.6772283368,-0.6533851828 H,0,2.6845173516,2.4942237878,-0.3846789382
Bn + X=Cl, Y=Cl	C,0,0.9719929509,-0.0001320515,-0.7713863747 C,0,2.2870623263,-0.0000934929,-0.4134559062 H,0,0.5304765502,0.9238305466,-1.1238361678 H,0,0.5306243081,-0.9240500965,-1.1241346336 C,0,-0.3350021673,-0.000584367,1.0690568042 H,0,0.0775716211,-0.9187619903,1.4739313719 H,0,0.077900353,0.9171915628,1.4745009736 C,0,-1.6852838786,-0.0001928854,0.5828761054 C,0,-2.3674816125,1.2126353135,0.3135543707 C,0,-3.6617302034,1.209807748,-0.1912613085 C,0,-4.3180029332,0.0006193536,-0.4480842176 C,0,-3.6622835346,-1.2089714981,-0.1917469241 C,0,-2.3680353684,-1.2125977531,0.3130668494 H,0,-1.8652446231,2.1554658697,0.5151223878 H,0,-4.1667747109,2.1520666326,-0.3839999594 H,0,-5.3299822056,0.0009292423,-0.8413030519 H,0,-4.1677616274,-2.1509206637,-0.3848626374 H,0,-1.8662328757,-2.1557404384,0.5142553416 Cl,0,3.1473054495,1.4698100203,-0.0496353619 Cl,0,3.1475186526,-1.4699837184,-0.0500934626
Bn + X=H, Y=CO₂Me	C,0,-0.5271859823,-0.448389006,0.95138705 C,0,0.6591575522,-0.7493911099,-0.9495673945 H,0,-0.3177812387,-1.4222399232,1.3804024822 H,0,0.1255550314,0.3592179498,1.2627967481 H,0,-0.0074274349,-1.5216682438,-1.3163536743 H,0,0.4162770312,0.2732274535,-1.2145540193 C,0,1.9456314987,-1.0532664393,-0.5943854655 H,0,2.2881078053,-2.0773207782,-0.4884146185 C,0,2.8841262282,0.0160193683,-0.244906767 O,0,2.6147537509,1.2056315673,-0.1792143932 O,0,4.1241052468,-0.4772489769,0.0177489209 C,0,5.1057273377,0.5050541694,0.3717954624 H,0,5.2442810316,1.2260654836,-0.4383326523 H,0,4.8050150895,1.0481703965,1.2718149404 H,0,6.0278186629,-0.0483358268,0.5506796162 C,0,-1.8660682762,-0.1469247968,0.535571741 C,0,-2.2479738571,1.1793722353,0.2122684718 C,0,-3.5376406567,1.4670671329,-0.2158417308 C,0,-4.4861615192,0.4451150368,-0.339455902

	C,0,-4.1291070591,-0.8721710165,-0.028916849 C,0,-2.8407384833,-1.166693782,0.3986445417 H,0,-1.514971901,1.9759624582,0.3088331119 H,0,-3.8105984198,2.4912928927,-0.4532441685 H,0,-5.49387499,0.6731128058,-0.673225307 H,0,-4.862450675,-1.668374021,-0.1199507024 H,0,-2.569422671,-2.1909221225,0.6417130731
Bn + X=Me, Y=CO2Me	C,0,2.9818917913,1.0856448814,0.4752676228 C,0,2.0572970562,0.0144970725,0.5601865249 C,0,2.496149325,-1.2688275607,0.1469811951 C,0,3.7901604009,-1.4668933486,-0.3172952329 C,0,4.6882065061,-0.3955250274,-0.3888469221 C,0,4.2749272118,0.8805804286,0.0111126514 C,0,0.7133253526,0.2250266577,1.0116501099 C,0,-0.5193744173,0.5911308659,-0.8638954955 C,0,-1.8120804303,0.8390963419,-0.4763603717 C,0,-2.6657067505,-0.3359052468,-0.209883825 O,0,-3.9451166375,0.0193105267,0.0865652558 C,0,-4.8319689473,-1.0739478719,0.3570698112 O,0,-2.2975598815,-1.5003237057,-0.235568453 H,0,0.4650143476,1.1599434071,1.502487364 H,0,0.1028113477,-0.6306889633,1.2764348663 H,0,0.118363126,1.4059922441,-1.188897637 H,0,-0.2473973513,-0.4055338368,-1.1882166206 C,0,-2.3496822618,2.2225524381,-0.2326049225 H,0,-4.9003404209,-1.7404254681,-0.506639195 H,0,-4.4828938877,-1.6533303246,1.2158864152 H,0,-5.8015990286,-0.6230198058,0.5692095707 H,0,1.8029497706,-2.1041027373,0.2018843769 H,0,4.1059946055,-2.4599925724,-0.6240128422 H,0,5.6994841134,-0.5534886662,-0.7511369222 H,0,4.9684899974,1.7152620052,-0.0389134689 H,0,2.6677316629,2.0784989505,0.7873436876 H,0,-2.6505715785,2.3636641643,0.8127244199 H,0,-1.6010723711,2.9798216889,-0.4805309163 H,0,-3.2444212027,2.4109275622,-0.8358843941
Bn + X=H, Y=CN	H,0,4.507563501,0.571188017,-0.8529927411 C,0,3.5140932358,0.3782215682,-0.4600130202 C,0,3.1063408364,-0.9337742314,-0.1923279831 H,0,3.7861205678,-1.7607848314,-0.3758203228 C,0,2.6357361168,1.4404322868,-0.2159881903 H,0,2.9492666627,2.4604178607,-0.4183293453

	C,0,1.3644702497,1.1972447974,0.287700822 H,0,0.6877267979,2.0258638597,0.4794440148 C,0,1.8362672692,-1.1836723187,0.3112288621 H,0,1.5263382923,-2.2040524067,0.5220837824 C,0,0.9317182806,-0.123137985,0.568929195 C,0,-0.3904971945,-0.3785445722,1.0598811655 H,0,-0.6224555125,-1.3576388862,1.4647946273 H,0,-0.9778629268,0.4438430589,1.4531048788 C,0,-1.690952624,-0.6155029129,-0.8028592775 H,0,-1.0863470248,-1.4533469948,-1.1296761778 H,0,-1.3735566476,0.3647203228,-1.1386011914 C,0,-2.9920221069,-0.830367411,-0.4218911868 C,0,-3.8973978569,0.2287110889,-0.1613939281 N,0,-4.649084194,1.0953409845,0.0557467017 H,0,-3.3597415889,-1.8352587514,-0.2338331892
Bn + X=H, Y=CHO	C,0,-1.5617326716,-0.4501324209,-0.8162758467 C,0,-2.8647849659,-0.640193211,-0.4328571842 H,0,-0.9502982585,-1.28142699,-1.1474760046 H,0,-1.2339913635,0.5330119173,-1.1430248056 C,0,-0.2594123664,-0.2856355235,1.0521356401 H,0,-0.7985942171,0.562770595,1.458258593 H,0,-0.5472169044,-1.254734756,1.4444333931 C,0,1.0767302231,-0.0969761366,0.5679479223 C,0,1.9183138153,-1.2031529837,0.2904600406 C,0,3.2025269829,-1.0178571035,-0.2051019043 C,0,3.6876284221,0.2731169161,-0.4443686119 C,0,2.872126855,1.3797602702,-0.180686611 C,0,1.5869170518,1.2009381201,0.3145920703 H,0,1.5480607677,-2.2075652718,0.4791315321 H,0,3.8332169202,-1.8793951602,-0.4042940575 H,0,4.6921512756,0.4154720453,-0.8307736637 H,0,3.2456675854,2.3835674533,-0.3609699501 H,0,0.9591337172,2.0637178905,0.5219008038 H,0,-3.259802057,-1.6332809442,-0.2333471082 C,0,-3.7705965392,0.4782472561,-0.2206825257 O,0,-4.9363764244,0.3736101071,0.135721278 H,0,-3.3236169126,1.4802912641,-0.4205868939
Bn + X=Me, Y=CN	C,0,1.3987944691,0.2290565232,-0.7730294716 C,0,2.7118704695,0.344438021,-0.3801515248 H,0,0.8664632151,1.1109041981,-1.1122771422 H,0,1.0106444911,-0.7244014727,-1.1104663813 C,0,0.0647154557,0.1140825737,1.0765775856

	H,0,0.5490878748,-0.7753244459,1.464391414 H,0,0.400253629,1.0549977558,1.499632576 C,0,-1.2742360185,0.0181423023,0.5728191304 C,0,-2.0481060661,1.1788782617,0.3218383681 C,0,-3.332674087,1.0840755971,-0.1979172919 C,0,-3.8865412464,-0.1680829686,-0.4884932435 C,0,-3.139052662,-1.3273842679,-0.2508930098 C,0,-1.8539644778,-1.2392367156,0.2688104473 H,0,-1.6250006361,2.1539155937,0.5500115024 H,0,-3.9102164192,1.9866160695,-0.3762276466 H,0,-4.8911563436,-0.2397517948,-0.8938268324 H,0,-3.5655266121,-2.3018453289,-0.4706723421 H,0,-1.2795521024,-2.1430038561,0.4550759745 C,0,3.3823937166,1.6655084796,-0.0923365729 H,0,4.3141693786,1.7667700012,-0.6596041664 H,0,2.7238645715,2.4953218461,-0.3610568823 H,0,3.6431227066,1.761069939,0.9687950473 C,0,3.4724935811,-0.835802239,-0.1340172444 N,0,4.1128124918,-1.7896174158,0.0724259778
Bn + X=H, Y=Ph	C,0,-3.7453129579,-1.0945472005,0.0584306527 C,0,-2.5014661735,-0.5290495803,-0.2957108148 C,0,-2.4221169863,0.8794795742,-0.3710536935 C,0,-3.5323185854,1.6744378377,-0.1089786606 C,0,-4.7566612136,1.0933761866,0.2364480797 C,0,-4.8557869708,-0.2975203381,0.3182326011 C,0,-1.3718699343,-1.4050433229,-0.562266028 C,0,-0.0989929455,-1.0270905157,-0.9069335605 C,0,1.0987940347,-0.6170914644,1.0070374249 C,0,2.3939786434,-0.1822803452,0.5724809132 C,0,2.660476707,1.185113455,0.3089199202 C,0,3.9066390426,1.599433649,-0.1441446464 C,0,4.9293765979,0.667407054,-0.3544951321 C,0,4.6880157259,-0.6882837334,-0.1033964497 C,0,3.4439167142,-1.1085194828,0.3496708306 H,0,0.3902583516,0.1157988151,1.3769318635 H,0,0.9874374357,-1.6191575868,1.4058404754 H,0,0.1188526277,-0.0208517445,-1.2478464088 H,0,0.6163606065,-1.7805600215,-1.21624477 H,0,1.8728446628,1.9159515294,0.4746247868 H,0,4.0876037993,2.6540071608,-0.3327951539 H,0,5.9028362534,0.9936419582,-0.7077293372 H,0,5.4781030963,-1.4173047002,-0.2606673556 H,0,3.2651533861,-2.1628248358,0.5454259735 H,0,-1.4816256417,1.3523125303,-0.6363743768

	H,0,-3.4449481279,2.7554844093,-0.1734521133 H,0,-5.6211319311,1.7180724036,0.440106459 H,0,-5.8008157585,-0.7610814705,0.5868954569 H,0,-3.8299669992,-2.1763510735,0.1254958411 H,0,-1.5609919522,-2.4660680133,-0.4056599622
Bn + X=Me, Y=Ph	C,0,-1.185781266,0.4197811788,1.0524854894 C,0,0.0465520451,0.904004818,-0.8260744235 H,0,-0.4975023301,-0.3425685166,1.4006273081 H,0,-1.0618687735,1.4013680215,1.4964318952 H,0,-0.1684017103,-0.0787708296,-1.2273225314 H,0,-0.6637448261,1.6741877786,-1.1052735745 C,0,1.3176412846,1.2658729133,-0.4423835762 C,0,-2.4829723544,0.0300584536,0.5832499735 C,0,-2.7753380604,-1.3202555992,0.2644991865 C,0,-4.0240358399,-1.6901598014,-0.2190010781 C,0,-5.0241522969,-0.7291417381,-0.406615461 C,0,-4.756991927,0.6106018388,-0.1017591442 C,0,-3.5103922386,0.9863592661,0.3823626005 H,0,-2.0059391655,-2.0739884036,0.4124601763 H,0,-4.2247558223,-2.7328283225,-0.4493902523 H,0,-5.9996884612,-1.0207055369,-0.7836313854 H,0,-5.5291686976,1.3621688605,-0.2411619626 H,0,-3.3121137397,2.0285342979,0.6200306335 C,0,1.6028099581,2.720639267,-0.1528450613 H,0,2.3778928046,3.1225231044,-0.8178373083 H,0,0.7049141456,3.3273895232,-0.2923546 H,0,1.95791936,2.874044145,0.8742083774 C,0,2.3920402315,0.283916921,-0.232370252 C,0,2.1638712948,-1.1094194979,-0.3095389769 C,0,3.1905176793,-2.0255158055,-0.1123669396 C,0,4.487380264,-1.5884403222,0.1726077824 C,0,4.7367529252,-0.2188961931,0.2598485413 C,0,3.7082356816,0.7002409933,0.0647635293 H,0,1.166909653,-1.4817028622,-0.5182037494 H,0,2.977706177,-3.0889847469,-0.1773023361 H,0,5.2880113206,-2.305495575,0.3270606414 H,0,5.738125998,0.1390322299,0.4823475017 H,0,3.9348797815,1.757916677,0.1381380262
tBu + X=H, Y=Me	C,0,-1.1170940926,0.1289129932,0.0643292573 C,0,0.7594907558,-0.9350204136,-0.6472142821

	H,0,0.2294473775,-1.8781191932,-0.5520118071 H,0,0.6697668348,-0.4408687144,-1.6119236341 C,0,1.8512784172,-0.6898521071,0.1388560916 H,0,2.0188277676,-1.3178294157,1.0133526809 C,0,-2.1145924186,-0.3498363499,-0.9578099535 H,0,-1.8350687527,-0.048081724,-1.9737123305 H,0,-2.2228165071,-1.4402926189,-0.943434292 H,0,-3.1152244782,0.0722826793,-0.7639836937 C,0,-0.7417711126,1.5844395561,-0.0211648495 H,0,-0.4805913936,1.8790091919,-1.0438337356 H,0,-1.5803093337,2.2287352727,0.2934935034 H,0,0.1063384004,1.8200582746,0.6296835757 C,0,-1.2883212062,-0.4168902332,1.4568625442 H,0,-2.1647005847,0.0304366701,1.9552472504 H,0,-1.4422287983,-1.5018210034,1.4525200213 H,0,-0.4148256045,-0.1996406109,2.0808125331 C,0,2.8154746888,0.4402143584,-0.0653330975 H,0,3.8473137284,0.0730392336,-0.154984857 H,0,2.5828502972,1.0078976821,-0.9718620613 H,0,2.814430856,1.1433874534,0.7794825837
tBu + X=Me, Y=Me	C,0,1.4297083914,0.0000041519,-0.1213794627 C,0,-0.4920878092,0.0000073018,1.0909831199 H,0,-0.1661787741,-0.9194303513,1.5696493836 H,0,-0.1661897741,0.9194512155,1.5696454889 C,0,-1.6404031259,-0.0000025418,0.3415429329 C,0,2.449158091,-0.0001128816,0.9883405991 H,0,2.3589667992,0.8870746367,1.6255714016 H,0,2.3588967363,-0.8873859759,1.625442025 H,0,3.4763549918,-0.000123138,0.5857053555 C,0,1.3384578155,1.2731596495,-0.920358979 H,0,1.2657889275,2.1556055838,-0.2746225432 H,0,2.2327227691,1.4117210092,-1.5518211676 H,0,0.4713782437,1.267896523,-1.5890376578 C,0,1.3383567862,-1.273036304,-0.9205300705 H,0,2.232600462,-1.4115749179,-1.5520272719 H,0,1.2656400922,-2.1555658286,-0.2749132793 H,0,0.4712639725,-1.2676227591,-1.5891903993 C,0,-2.2905869336,1.2772235081,-0.1183410943 H,0,-3.3370368141,1.3300890453,0.2152665806 H,0,-1.7709904479,2.1610278403,0.2620242911 H,0,-2.3186769701,1.3489876676,-1.2153545336 C,0,-2.2905798821,-1.277240415,-0.1183180667 H,0,-1.7709482884,-2.161035343,0.2620210887 H,0,-3.337013472,-1.3301289395,0.2153375941

	H,0,-2.3187184527,-1.3490010813,-1.2153302285
tBu + X=Me, Y=OMe	C,0,-1.8059961309,-0.133054744,0.143452035 C,0,0.0432514414,0.2897441716,-1.1548717691 H,0,-0.1658961081,-0.6251239443,-1.6971834844 H,0,-0.3981258324,1.2030272776,-1.5358967387 C,0,1.1982587698,0.3741269964,-0.4281724549 C,0,-2.9070021463,0.0012906784,-0.8751600317 H,0,-2.9663349049,1.0177227014,-1.2816054996 H,0,-2.7714395251,-0.6925428954,-1.7131853408 H,0,-3.8936561302,-0.2230195861,-0.4338614751 C,0,-1.7477639531,0.9435175577,1.1934361386 H,0,-1.8043282715,1.9464143817,0.7544237784 H,0,-2.5883629813,0.858477251,1.9039809814 H,0,-0.8263904085,0.8798508865,1.7822509504 C,0,-1.5270034966,-1.5305772923,0.6304105133 H,0,-2.3159994172,-1.8789175806,1.3196954555 H,0,-1.4874660024,-2.2476727319,-0.1972487108 H,0,-0.5744624861,-1.5866178062,1.1667714995 C,0,1.74334945,1.6464241012,0.1549416236 H,0,2.7653186344,1.8610229894,-0.1833603447 H,0,1.1150191167,2.4886402008,-0.141352169 H,0,1.7703549653,1.6154112615,1.2528484786 O,0,1.7891186897,-0.8214484723,-0.0646481018 C,0,3.1921387813,-0.8343058035,0.1510287737 H,0,3.7444352702,-0.5208182172,-0.7454090779 H,0,3.4942686752,-0.198890088,0.992936771 H,0,3.4547195945,-1.8683703135,0.3829907695
tBu + X=H, Y=Cl	C,0,-1.491379736,0.1772647278,0.0730653039 C,0,0.3224633487,-1.0310834543,-0.6886594679 H,0,-0.2755727796,-1.9351684581,-0.6321655637 H,0,0.2875430004,-0.4753772803,-1.618954605 C,0,1.4074815758,-0.9478050152,0.1237534124 H,0,1.5814162473,-1.5844976285,0.9816991555 C,0,-2.5307745143,-0.2429152933,-0.9316735495 H,0,-2.2403960725,0.020257513,-1.9550585186 H,0,-2.7244757011,-1.3208188878,-0.8957413099 H,0,-3.4925386968,0.2599618325,-0.7353442569 C,0,-1.6580432034,-0.3580897311,1.4690288066 H,0,-2.4896069786,0.1471323447,1.987742522 H,0,-1.8844090228,-1.4301576799,1.4716847723 H,0,-0.757500257,-0.1951925434,2.0703048819 C,0,-1.0015219193,1.5959585809,-0.0333473666

	H,0,-0.7597806619,1.8689369307,-1.0662431586 H,0,-1.7753344278,2.3022496686,0.3124552343 H,0,-0.1119689093,1.7647858513,0.5809290379 Cl,0,2.6090159383,0.3187005558,-0.0337830015
tBu + X=Me, Y=Cl	C,0,1.7143350167,-0.0971499023,-0.1380260404 C,0,-0.1777371302,0.2617273666,1.1219975023 H,0,0.0057559498,-0.6790307693,1.626922109 H,0,0.290072762,1.1445291928,1.5468852991 C,0,-1.3163279388,0.4406413653,0.3955160558 C,0,2.7445499582,-0.1776038312,0.957439163 H,0,2.8063698239,0.7531170229,1.5329736293 H,0,2.5364980849,-0.9977796629,1.6537056266 H,0,3.749274594,-0.3614885839,0.5411327842 C,0,1.7703443016,1.1297331226,-1.0074326855 H,0,1.8470577368,2.0486798838,-0.4152424817 H,0,2.65116184,1.1029859918,-1.671008332 H,0,0.8879488999,1.2074451137,-1.650754797 C,0,1.4017796633,-1.3879604907,-0.8452319543 H,0,1.2377762206,-2.2103080758,-0.1406206112 H,0,0.5115043922,-1.299510683,-1.4751527875 H,0,2.2371971263,-1.6878220219,-1.5007568589 Cl,0,-2.2735318831,-0.9783096224,-0.0668154854 C,0,-1.8354196828,1.7309554026,-0.1543939399 H,0,-2.8630988135,1.918094782,0.1794750919 H,0,-1.2060197238,2.5603616141,0.1804115048 H,0,-1.8506020097,1.7299315781,-1.2513155303
tBu + X=Cl, Y=Cl	C,0,-1.947288727,-0.0001380598,-0.1730597909 C,0,-0.0120735473,-0.0002486321,1.1590666248 H,0,-0.3517959791,0.9274597238,1.6026821699 H,0,-0.3516282257,-0.9282295542,1.6022473053 C,0,1.1537362352,-0.0000027257,0.4643399338 C,0,-2.987209244,-0.0001134904,0.914645006 H,0,-2.9154377209,-0.888587047,1.5521407664 H,0,-2.9154155537,0.8883811696,1.5521047162 H,0,-4.0032939213,-0.0001092036,0.4855226662 C,0,-1.795389783,-1.2767705162,-0.9526131088 H,0,-0.8917772636,-1.2701878926,-1.5697569433 H,0,-1.7577239324,-2.1550471497,-0.2991713517 H,0,-2.6510038351,-1.4214476112,-1.6340686456 C,0,-1.7952512966,1.2765122994,-0.9525566232 H,0,-1.757612086,2.1547676264,-0.2990860276 H,0,-0.8915746417,1.2699052389,-1.5696080358

	H,0,-2.6507859408,1.4212470539,-1.6340995388 Cl,0,1.9246629973,1.4699789782,-0.0744311674 Cl,0,1.9246844895,-1.4696016608,-0.0754417344
tBu + X=H, Y=CO2Me	C,0,2.0870863392,0.2250323453,0.2041585049 C,0,0.4239357417,-0.7026286978,-1.2210082539 H,0,0.2691339013,0.2890685019,-1.6291861428 H,0,1.2160805012,-1.297378764,-1.6626930099 C,0,-0.5603254887,-1.3053984226,-0.4978729419 H,0,-0.4851020687,-2.3444124306,-0.1940021575 C,0,1.2471544546,0.9703842649,1.2009445293 H,0,1.8871619693,1.475907777,1.9435524948 H,0,0.6299525747,1.7367751836,0.7234067353 H,0,0.5861214792,0.2941445843,1.7515594335 C,0,2.7695326944,-1.0179027556,0.702908543 H,0,3.2358783201,-1.5863042873,-0.1090257361 H,0,3.5721170809,-0.7595363423,1.4140516576 H,0,2.0730422784,-1.6757882899,1.232753292 C,0,2.835753868,1.0479484021,-0.8063769119 H,0,3.2373815374,0.433950731,-1.6201357646 H,0,2.2075375632,1.8324742558,-1.2410674791 H,0,3.6963649686,1.5525509228,-0.3354081546 C,0,-1.7794159652,-0.640510222,-0.026726211 O,0,-2.6571263356,-1.1888366273,0.6181165826 O,0,-1.8492716697,0.6728038897,-0.3918170249 C,0,-3.037370281,1.3526753139,0.0309698689 H,0,-2.9366735085,2.3770673971,-0.3289638908 H,0,-3.9273551168,0.8841614615,-0.3975284587 H,0,-3.128565616,1.3379798312,1.1203079552
tBu + X=Me, Y=CO2Me	C,0,-2.1306808913,-0.4242427327,0.227644584 C,0,-0.4492076924,0.4883096539,-1.1846181376 C,0,0.5592086021,1.0717243722,-0.4704556658 H,0,-1.2271388058,1.1049033429,-1.6230567207 H,0,-0.3184304109,-0.5032867694,-1.5983483147 C,0,-1.3085247151,-1.1332112647,1.2655347069 H,0,-0.6458194251,-1.8797145247,0.8188457833 H,0,-0.6931552203,-0.4319953017,1.8380715453 H,0,-1.9594878547,-1.6560480698,1.986652671 C,0,-2.8629965205,0.8079779149,0.6818308373 H,0,-2.2097139012,1.4882456211,1.2373870922 H,0,-3.3035508765,1.3577930694,-0.1571146676 H,0,-3.6935569264,0.5389072378,1.356731238 C,0,-2.8380357636,-1.2867818885,-0.7805908125

	H,0,-2.1881833281,-2.076908271,-1.1710403435 H,0,-3.7091878927,-1.7858843778,-0.3230545848 H,0,-3.2181847839,-0.7022293082,-1.6259587178 C,0,1.7475688581,0.3072286262,-0.0447057233 O,0,2.6800877666,0.784837778,0.5809359469 O,0,1.7227411336,-1.0028390216,-0.4253067124 C,0,2.8784169311,-1.7609067871,-0.0476510793 H,0,3.0033964235,-1.766517333,1.0383861256 H,0,2.7026362579,-2.7719660853,-0.4163441287 H,0,3.7825299771,-1.3427909891,-0.4981847067 C,0,0.540183897,2.5133764298,-0.0379645599 H,0,0.5615899383,2.6052261816,1.0541438008 H,0,1.4280468422,3.0418122202,-0.4020656619 H,0,-0.3500174474,3.0236173616,-0.4142291848
tBu + X=H, Y=CN	C,0,-1.3959522711,0.2210232554,0.0707392605 C,0,0.4568339811,-1.132743121,-0.6958916012 H,0,-0.2018951998,-1.9905360563,-0.6278252233 H,0,0.4195045695,-0.5547298923,-1.6118492158 C,0,1.5197376596,-1.0292304147,0.1518598105 H,0,1.6223336299,-1.6985725715,1.001404335 C,0,-2.4349718683,-0.2031414005,-0.9278685355 H,0,-2.1296072519,0.0173638577,-1.9565114373 H,0,-2.6646890353,-1.2717590145,-0.8546620927 H,0,-3.3815955235,0.3368951549,-0.7568821376 C,0,-0.8099107932,1.5938929941,-0.0907679543 H,0,-0.5994203168,1.8306597232,-1.1388229703 H,0,-1.5140709702,2.3598037387,0.2757531084 H,0,0.1158634549,1.7113007176,0.4810462082 C,0,-1.5507251819,-0.2830479994,1.4765981281 H,0,-2.3515778554,0.2658390302,1.9996774378 H,0,-1.8203524005,-1.3442544516,1.5057810896 H,0,-0.6338764203,-0.1404453539,2.0575771143 C,0,2.5125259693,-0.0211884272,0.026769152 N,0,3.3363083353,0.8007208282,-0.0633308253
tBu + X=H, Y=CHO	C,0,-1.4339106657,-0.1635183974,-0.1441988812 C,0,0.5310118835,0.9079868679,0.9391441036 H,0,-0.1470895031,1.7023497084,1.2292627711 H,0,0.559344206,0.0184768692,1.5585712471 C,0,1.5277925136,1.1169877498,0.039158111 H,0,1.6010328368,2.0493285161,-0.5162089858 C,0,-2.124213695,-0.6443344108,1.0988536181 H,0,-1.5250533073,-1.384056751,1.6394731973

	H,0,-2.361777857,0.1788869543,1.782000721 H,0,-3.0819336149,-1.1321372444,0.8480348649 C,0,-0.7417320636,-1.1878712922,-0.9920518087 H,0,-0.1070039829,-1.8517657685,-0.3985053726 H,0,-1.4801738013,-1.8163611455,-1.5189920094 H,0,-0.1155825092,-0.7186324557,-1.7571388196 C,0,-2.032946205,1.0179346533,-0.850254262 H,0,-2.9158937809,0.7136894244,-1.4381990697 H,0,-2.3698285728,1.7899647734,-0.1501905032 H,0,-1.3240941943,1.4689566455,-1.5524298937 C,0,2.5378377462,0.0919980616,-0.2319002578 O,0,2.5425457421,-1.0315223643,0.2568725377 H,0,3.3446510602,0.3983799946,-0.9331621865
tBu + X=Me, Y=CN	C,0,-1.6427011485,0.1395231369,0.1423931335 C,0,0.3140670764,-0.3484186151,-1.157714825 H,0,-0.1799109344,-1.2491032143,-1.5059528804 H,0,0.1004528953,0.5677274579,-1.6949733952 C,0,1.4361629523,-0.4546216531,-0.3823073694 C,0,-2.6895637446,-0.0370187029,-0.9217017591 H,0,-2.5280502971,0.6361066833,-1.7708486785 H,0,-2.7259891278,-1.0656686639,-1.2967046068 H,0,-3.6926172789,0.1915482318,-0.5234959927 C,0,-1.3444146076,1.5474829469,0.5736822231 H,0,-1.281159046,2.2332545491,-0.2776629139 H,0,-2.1428642746,1.9279658648,1.2329297432 H,0,-0.40743644,1.6127543918,1.1357323211 C,0,-1.5771218997,-0.9146848468,1.2104899367 H,0,-2.4245566951,-0.8140657994,1.9096877869 H,0,-1.6281293481,-1.9263892686,0.7938955909 H,0,-0.6627105994,-0.8292621316,1.8058649324 C,0,1.9177502716,-1.752360758,0.2236384579 H,0,1.2681363942,-2.5782302589,-0.0763862632 H,0,2.9392268102,-1.9819888007,-0.1006926392 H,0,1.9334888586,-1.7068206062,1.318592159 C,0,2.1913431012,0.7168849182,-0.0735650051 N,0,2.8284267251,1.6573504298,0.1943608686
tBu + X=H, Y=Ph	C,0,2.6750755944,0.1683358048,0.3435103558 C,0,1.1201687401,-0.4650041924,-1.3680007073 H,0,1.0912622044,0.5738632902,-1.6798659 H,0,1.9244106454,-1.0586325558,-1.7878143474 C,0,0.0231117046,-1.0874653606,-0.8467647252 H,0,0.081335684,-2.1627493267,-0.6836365263

	C,0,3.7423471101,0.7984682176,-0.5069117016 H,0,4.1700770462,0.0868161472,-1.2221136252 H,0,3.3632556232,1.6613749939,-1.0660272929 H,0,4.5782046023,1.1654971634,0.1136087662 C,0,2.9976537254,-1.1679067796,0.951170314 H,0,3.4630754842,-1.8458363059,0.2271163433 H,0,3.7066142549,-1.0594725372,1.7898481632 H,0,2.1011555866,-1.6538014323,1.3503789603 C,0,1.844684184,1.0942912827,1.1857019673 H,0,2.4058463969,1.4275328107,2.0760116197 H,0,1.5537749387,1.9964869673,0.6370320188 H,0,0.9338075806,0.6043791282,1.5439843166 C,0,-1.2310106326,-0.4711159536,-0.4278095762 C,0,-2.229017934,-1.2752842094,0.1618635372 C,0,-3.4476035241,-0.739066179,0.5684904949 C,0,-3.708231887,0.6219543602,0.3975377097 C,0,-2.7337431425,1.4365306545,-0.188137143 C,0,-1.516578023,0.9016572101,-0.5954421673 H,0,-2.0350522978,-2.3363444511,0.2986393067 H,0,-4.1959260429,-1.384421171,1.0200722741 H,0,-4.6576254768,1.0437186019,0.7135943472 H,0,-2.9271274601,2.4964045247,-0.3293658121 H,0,-0.7782242627,1.5528150199,-1.0527127615
tBu + X=Me, Y=Ph	C,0,2.6227623226,-0.5016450873,0.3523272817 C,0,1.0937541384,0.3799689711,-1.2532991833 H,0,1.9253649256,0.9586366285,-1.6403701151 H,0,1.0035020668,-0.6233554739,-1.6515360572 C,0,0.0326537335,1.0286711743,-0.6765502647 C,0,3.5687775855,-1.2175436265,-0.5719727541 H,0,3.0700804649,-2.0196986831,-1.1272951703 H,0,4.0307661735,-0.5355930011,-1.2950636026 H,0,4.3930644173,-1.6872582898,-0.0078930452 C,0,1.7362418984,-1.3621917964,1.2075235932 H,0,1.2978239034,-2.1902973685,0.6410796491 H,0,2.3066228797,-1.8088839399,2.0405193816 H,0,0.9187770366,-0.7847570795,1.6506702377 C,0,3.1460195506,0.7507319852,0.9995065715 H,0,3.886860299,0.5104847202,1.7817739319 H,0,3.6475315182,1.4062339559,0.2788937671 H,0,2.3447681757,1.3193297493,1.4820081399 C,0,-1.2340090795,0.3541667046,-0.3355670718 C,0,-2.2491547904,1.0335324344,0.3724881468 C,0,-3.4558447545,0.4145095952,0.6946748591 C,0,-3.6958539557,-0.9064534778,0.3194623913

	C,0,-2.7079641246,-1.5991356753,-0.3871560215 C,0,-1.5048207842,-0.9824796553,-0.7084973607 H,0,-2.0957539673,2.0614223895,0.6808746952 H,0,-4.2111923282,0.9709499137,1.2428302367 H,0,-4.6358539348,-1.3894126536,0.5689371907 H,0,-2.8794215546,-2.6273753814,-0.6937808396 H,0,-0.7660381943,-1.5471668716,-1.266421542 C,0,0.1712820689,2.4957394623,-0.336909827 H,0,1.1364368857,2.8823630682,-0.6719399128 H,0,-0.6146636593,3.0962056682,-0.8121354853 H,0,0.0982620381,2.6809465976,0.7426663772
MOH + X=H, Y=Me	C,0,1.4493894985,-0.4944462528,0.4151154112 C,0,-0.3045146066,0.8509044298,-0.2612634227 H,0,1.4706651216,-0.2739711581,1.4829124161 H,0,1.0598451996,-1.4668888393,0.1320219295 H,0,0.24558343,1.7189676118,0.0906551499 H,0,-0.0771846162,0.5316254751,-1.2746710191 C,0,-1.4823966516,0.5019169298,0.3276399959 H,0,-1.7507782575,0.9580310216,1.2801891303 O,0,2.5720876335,-0.174862372,-0.3134551996 H,0,2.9444743766,0.6459570474,0.0334547849 C,0,-2.4090006165,-0.5569010837,-0.1912107159 H,0,-3.4309316999,-0.1732562529,-0.3131271551 H,0,-2.0769449349,-0.9387868534,-1.1621105388 H,0,-2.4822954295,-1.4116232143,0.4966292884
MOH + X=Me, Y=Me	C,0,-1.7947147681,0.0066170777,0.6392150815 C,0,-0.0279260553,-0.0534560518,-0.852076561 H,0,-1.6470309008,-0.9290137963,1.180330679 H,0,-1.5645211544,0.9170844951,1.1832421817 H,0,-0.4089543683,-0.9934572095,-1.2427998767 H,0,-0.4524721284,0.8435603753,-1.2918992479 C,0,1.1873688366,-0.0163799486,-0.2301604722 O,0,-2.9651774476,0.1363840514,-0.0751750468 H,0,-3.181240704,-0.7168224424,-0.4726787338 C,0,1.842974507,1.2845797307,0.1479953588 H,0,2.8628893919,1.3495252584,-0.2563412414 H,0,1.2797951449,2.1473040034,-0.2192036682 H,0,1.9411591173,1.3863729441,1.2390561029 C,0,1.8942814206,-1.2703076154,0.2093551196 H,0,1.3676485696,-2.1723963639,-0.115907942

	H,0,2.9164344377,-1.3134592359,-0.1922750299 H,0,1.9958085307,-1.3160895952,1.3039059899
MOH + X=Me, Y=OMe	C,0,-2.2300697458,-0.0931620112,-0.6305105589 C,0,-0.4923128429,0.2254246789,0.8975388881 H,0,-2.2291362165,0.854420207,-1.1604736709 H,0,-1.8316633208,-0.9517868492,-1.1713477929 H,0,-0.9874776262,1.1204991488,1.251391923 H,0,-0.7735089208,-0.7131263161,1.3610924455 C,0,0.7146546936,0.3202508992,0.2733468626 C,0,1.2999764361,1.6027033657,-0.2445096902 H,0,0.655376194,2.4418047885,0.0256750546 H,0,2.2978352149,1.8088806394,0.1627167561 H,0,1.3978551937,1.5877546923,-1.3390424262 O,0,1.3246653368,-0.8685065085,-0.0851924058 C,0,2.7432703179,-0.8951747592,-0.1194894544 H,0,3.023772992,-1.9216639143,-0.3648028319 H,0,3.15843572,-0.227354771,-0.8851055802 H,0,3.179314751,-0.6311005417,0.8538973369 O,0,-3.4114562396,-0.2769408164,0.0566575596 H,0,-3.4095899121,-1.1650015249,0.4360212727
MOH + X=H, Y=Cl	C,0,1.8840130641,-0.2920556557,0.5725641552 C,0,0.1534050931,0.9703036288,-0.4097802279 H,0,2.0474521495,0.3020657661,1.4652794093 H,0,1.3439246733,-1.2301451852,0.6893480734 H,0,0.7345711092,1.8709079978,-0.2439572802 H,0,0.3503713189,0.4219908964,-1.3236442949 C,0,-1.0169630375,0.8244296202,0.2524518034 H,0,-1.3313600993,1.4325164311,1.0909012678 O,0,2.9784987137,-0.284433635,-0.25177292 H,0,2.8498032578,-0.9357619586,-0.9535316079 Cl,0,-2.1144401669,-0.5060100251,-0.0706839172
MOH + X=Me, Y=Cl	C,0,2.0902513276,0.0557918475,-0.6396879155 C,0,0.3330929933,0.3411786233,0.8945298184 H,0,1.6657444728,-0.7561493277,-1.2283516867 H,0,2.1057466331,1.0407677152,-1.0944452824 H,0,0.6676713448,-0.5742051247,1.3665845881 H,0,0.7976048497,1.261606191,1.2318151015 C,0,-0.875205453,0.4081134579,0.2817619508 O,0,3.2461279378,-0.1993716676,0.0542425066 H,0,3.2530863677,-1.1275814534,0.3215801537

	Cl,0,-1.7256631535,-1.1037408654,-0.0929296104 C,0,-1.5428156497,1.6352992106,-0.2506308698 H,0,-2.5606670732,1.7369418689,0.1432592134 H,0,-0.9717720096,2.5237681839,0.0343960361 H,0,-1.6221037873,1.6111211635,-1.3448127025
MOH + X=Cl, Y=Cl	C,0,2.3197518772,-0.0002142008,-0.7256224912 C,0,0.5626532441,-0.0000740718,0.8923980686 H,0,2.0813348407,-0.9359806733,-1.2300646935 H,0,2.0814004645,0.9355174288,-1.2301622429 H,0,0.9888720832,-0.9269081021,1.2541590145 H,0,0.9890463016,0.9266545768,1.2542162446 C,0,-0.6670040173,0.0000254547,0.3361058004 O,0,3.3627447073,-0.0002332873,0.169714877 H,0,4.2150989259,0.0009160205,-0.2922224086 Cl,0,-1.4866582048,1.4696911939,-0.1214757233 Cl,0,-1.4868780833,-1.4695003731,-0.1215203471
MOH + X=H, Y=CO2Me	C,0,-2.2236569582,-0.0129686207,-0.556855028 C,0,-1.4479904893,1.0203189151,0.3350229557 H,0,-2.9061709782,0.5185132261,-1.2263866289 H,0,-1.5105223922,-0.5683173191,-1.1785845972 H,0,-1.9853854349,1.9714776264,0.3711650616 H,0,-1.4556317241,0.5992880826,1.3481813006 C,0,-0.0386448313,1.2217908753,-0.0888737049 H,0,0.3086345654,2.1400041199,-0.5503792761 C,0,0.9011479458,0.1308094623,0.0857154691 O,0,0.606903314,-0.966747496,0.55015602 O,0,2.1548017252,0.4515450676,-0.327116627 C,0,3.128902073,-0.5911128915,-0.1826388463 H,0,4.0657219495,-0.173238052,-0.5508392174 H,0,3.2274462139,-0.8874713939,0.8650589424 H,0,2.8456011238,-1.4700625575,-0.7679398037 O,0,-3.023495437,-0.8917326493,0.2103681455 H,0,-2.4139165812,-1.4877395527,0.668238836
MOH + X=Me, Y=CO2Me	C,0,3.2412665429,-0.8205048219,-0.4050516968 O,0,2.229067258,0.1847119881,-0.2676009022 C,0,1.0524524758,-0.2510339592,0.2609999239 O,0,0.8730917954,-1.4133643588,0.586155464 C,0,0.0598635912,0.8408463008,0.3711172382 C,0,0.37897515,2.1954645958,-0.2055029842 C,0,-1.1282303506,0.5360706368,0.9563888641

	C,0,-2.6048056031,-0.5112331536,-0.7271679755 O,0,-3.8369021529,-0.789593654,-0.2092753066 H,0,-1.8710890621,1.3056998883,1.1385456278 H,0,-1.2599356191,-0.4147129904,1.4567232581 H,0,-4.3952403746,-0.0039455461,-0.2738785184 H,0,4.1030642837,-0.3154693655,-0.8420835689 H,0,3.5002519009,-1.2460734168,0.5680107049 H,0,2.8997403508,-1.628948574,-1.0568639684 H,0,1.2747388291,2.6236663382,0.2571967139 H,0,0.5847248451,2.1420879657,-1.2810562236 H,0,-0.4524173322,2.8883838743,-0.048514228 H,0,-1.96888453,-1.3855682376,-0.7889586093 H,0,-2.5341393333,0.2431906697,-1.5080554483
MOH + X=H, Y=CN	C,0,-1.8103427749,-0.0762315826,0.6886957344 C,0,-0.0727518571,1.54250718,0.0003969587 H,0,-1.3855859998,-0.2814155406,1.6686809399 H,0,-2.7591199917,0.447587954,0.630505745 H,0,-0.5446288373,1.3070556839,-0.9450418365 H,0,-0.4194216649,2.430063085,0.5188295447 C,0,1.0885587181,0.9400877841,0.3782408774 H,0,1.6289746627,1.2516880972,1.2669907991 O,0,-1.6621506105,-0.9996627912,-0.2932902039 H,0,-0.8117035757,-1.4564663827,-0.1980620258 C,0,1.5470410781,-0.2390516545,-0.2677641438 N,0,1.867665615,-1.2435829899,-0.7704282994
MOH + X=H, Y=CHO	C,0,-1.7559413605,0.02635092,-0.5624014632 C,0,0.1696630845,0.2843707221,1.2090918367 H,0,-1.8352626969,1.0829486524,-0.8040640373 H,0,-1.0682572142,-0.6012531298,-1.1139792767 H,0,-0.4850688926,0.77699051,1.9197765128 H,0,0.0977500808,-0.7938914186,1.1273738279 C,0,1.1722182158,0.943065121,0.583954325 H,0,1.3242664702,2.0108207717,0.7252769199 O,0,-2.866029872,-0.6336507535,-0.1331368864 H,0,-3.481993653,-0.0043750182,0.2644667211 C,0,2.0738727713,0.2500374126,-0.3435033255 O,0,1.9370744522,-0.910595552,-0.7062925192 H,0,2.9213329977,0.8597850228,-0.7262636603
MOH + X=Me, Y=CN	C,0,-2.9532627213,-1.0422969627,-0.8169232449

	C,0,0.0739799624,1.439451072,0.9591249759 H,0,-3.9366218626,-0.7370462964,-0.47853891 H,0,-2.8510783941,-1.6653119073,-1.7017708515 H,0,0.1312513842,2.4196384182,1.4237191082 H,0,-0.8675168043,0.9018186998,1.0067356092 C,0,1.1441514501,0.9142925122,0.3421026696 O,0,-2.0544620919,-1.205094397,0.2021700202 H,0,-1.2297033464,-1.5734546474,-0.1537738067 C,0,0.9984129316,-0.386293946,-0.2514595751 N,0,0.8697735238,-1.4450402408,-0.7199688187 C,0,2.4981093783,1.59169404,0.223606526 H,0,2.9162769461,1.7921582797,1.2144863245 H,0,3.210115236,0.9713319588,-0.3234476341 H,0,2.4062129032,2.5458220631,-0.3036963788
MOH + X=H, Y=Ph	C,0,3.0621691002,-0.2274473713,-0.8390824332 C,0,1.7270104198,0.8509588187,0.9124850747 H,0,2.2726837366,-0.8697163343,-1.2113398622 H,0,3.3200589402,0.6519418442,-1.4268437217 H,0,1.809176512,-0.1138726467,1.4004177703 H,0,2.544769992,1.539781932,1.0948286396 C,0,0.5544107376,1.310730417,0.3989914633 H,0,0.5186888784,2.3417064845,0.0494005006 O,0,4.0849132409,-0.9392415196,-0.2693355287 H,0,4.8039681153,-0.3340636789,-0.0466437155 C,0,-0.6769596249,0.5506258981,0.2029726588 C,0,-1.8157093807,1.2034229318,-0.3109346695 C,0,-3.0136457628,0.5226481616,-0.5109471643 C,0,-3.1079214758,-0.8366422253,-0.2062504773 C,0,-1.9880472582,-1.5036870156,0.2997980446 C,0,-0.7912409722,-0.8238901185,0.5009795631 H,0,-1.7510839882,2.261864795,-0.5513399428 H,0,-3.8751755625,1.0533290124,-0.9066633753 H,0,-4.0401619207,-1.3712444231,-0.3622676987 H,0,-2.0491687493,-2.5623207259,0.5369363996 H,0,0.0665434214,-1.3637910811,0.8901268739
MOH + X=Me, Y=Ph	C,0,-2.9522600633,-0.6198299615,-0.776918209 C,0,-1.6957782487,0.6440075531,0.8771695128 H,0,-3.6113799874,0.1584457245,-1.1597774003 H,0,-2.1134593957,-0.9180236571,-1.3948296448 H,0,-2.553735159,1.2837709162,1.0569092498 H,0,-1.695558744,-0.3015493824,1.4053897112 C,0,-0.5596646551,1.1713490265,0.3331103858

	O,0,-3.53392655,-1.691790408,-0.1481631736 H,0,-4.3271445704,-1.3925507203,0.3145947746 C,0,-0.5660135232,2.596833351,-0.168830325 H,0,-1.5636728759,3.0352629705,-0.0839654922 H,0,0.1195226925,3.2337009799,0.4053376993 H,0,-0.2533854647,2.6640618774,-1.218342158 C,0,0.6743517671,0.3787021057,0.1730739269 C,0,0.6811016912,-1.0265165338,0.3184881574 C,0,1.8509556143,-1.7642062767,0.1707628829 C,0,3.0578161403,-1.128733944,-0.1338801053 C,0,3.0725027135,0.256722499,-0.2937834087 C,0,1.9006161979,0.996991092,-0.1478975147 H,0,-0.2453963291,-1.5501761857,0.5290388854 H,0,1.8192862145,-2.8443362364,0.2848173052 H,0,3.9696859697,-1.7066605508,-0.2513593845 H,0,4.0009250846,0.7673182064,-0.5346239909 H,0,1.94395916,2.073145853,-0.275655984
POH + X=H, Y=Me	C,0,-1.1288450701,0.1116977793,0.0286786524 C,0,0.782355452,-0.8077518618,-0.7662201053 H,0,0.2599548166,-1.7580148857,-0.8467275134 H,0,0.6889015259,-0.1545073399,-1.6303662135 C,0,1.86557182,-0.7029252228,0.0623516274 H,0,2.0330363846,-1.4784458337,0.8094205552 C,0,-0.8029530838,1.566018007,0.18271491 H,0,-0.5492808116,2.0094939029,-0.7847403883 H,0,-1.6582941055,2.1276616747,0.5901187257 H,0,0.043725538,1.697468891,0.8613788726 C,0,-1.4052644667,-0.6871648673,1.2716321288 H,0,-2.3094889601,-0.3321324381,1.7909144076 H,0,-1.5528679934,-1.7504786422,1.0413067825 H,0,-0.5633172476,-0.6158222992,1.9659501521 O,0,-2.0195670945,-0.078952575,-1.0177480773 H,0,-2.271748416,-1.0121172071,-1.0401389544 C,0,2.8199659738,0.4547240575,0.0766021758 H,0,3.8563746439,0.1216053859,-0.0741736459 H,0,2.584880455,1.1773915061,-0.7113287862 H,0,2.8096771748,0.9919305338,1.0358142898
POH + X=Me, Y=Me	C,0,1.4450778846,0.0149107981,-0.0701064279 C,0,-0.5103649074,-0.0325161905,1.0667889288 H,0,-0.1952272759,-0.9664601189,1.5278181353

	H,0,-0.1743815761,0.8687110317,1.5714326555 C,0,-1.654919677,-0.0119936936,0.3110592532 C,0,1.4001423511,1.2947514547,-0.8488250639 H,0,1.3113697331,2.1530662898,-0.1761656811 H,0,2.3165795125,1.4343484689,-1.4436948741 H,0,0.5480562636,1.2972178528,-1.5335031031 C,0,1.4613806652,-1.2781075027,-0.8379217612 H,0,2.3875886842,-1.3890398507,-1.4245636574 H,0,1.3906646294,-2.144797851,-0.1676871362 H,0,0.6156923525,-1.3269542811,-1.5290501648 O,0,2.3773404381,0.1074194398,0.9555700616 H,0,2.4355413906,-0.7517292952,1.3952736657 C,0,-2.304169995,-1.2756841799,-0.1868394326 H,0,-1.7984055116,-2.1706558215,0.1873296503 H,0,-3.3577032889,-1.329895595,0.1237491052 H,0,-2.3113420732,-1.3287443324,-1.285822616 C,0,-2.2958108567,1.2782892757,-0.125570937 H,0,-3.3473486919,1.3259278614,0.1929682997 H,0,-1.7803192797,2.1502487468,0.2866778813 H,0,-2.3075011626,1.3815016061,-1.2208300087
POH + X=Me, Y=OMe	C,0,1.8268182397,-0.1146222582,-0.0910144585 C,0,-0.0703351479,0.2456227665,1.1413513942 H,0,0.1194666017,-0.6909729086,1.6552314723 H,0,0.383664215,1.1354001232,1.5607152265 C,0,-1.2134024502,0.3616567789,0.4008680831 C,0,1.8937554592,1.056676804,-1.0223767098 H,0,1.9846282193,1.9923356896,-0.4619559906 H,0,2.7639972598,0.9896984032,-1.6950200151 H,0,0.9934001106,1.1042532318,-1.6407385982 C,0,1.5873114884,-1.4769543671,-0.6796345131 H,0,2.4120571315,-1.7869026736,-1.3425585978 H,0,1.4915957217,-2.2394279817,0.104448227 H,0,0.657977881,-1.4894755857,-1.2547271261 O,0,2.8424075225,-0.0394621491,0.8556954587 H,0,2.8178290696,-0.8441209028,1.3910555219 C,0,-1.7431864701,1.652769497,-0.1543246641 H,0,-2.7699269042,1.8632633767,0.1726113337 H,0,-1.1174585417,2.4844889194,0.1759636307 H,0,-1.7540204436,1.6517112779,-1.2533733847 O,0,-1.7981125966,-0.82008192,-0.0273736155 C,0,-3.2107687723,-0.8397224401,-0.1651936578 H,0,-3.5670210534,-0.1554719375,-0.945927382 H,0,-3.4769117927,-1.8600547391,-0.4493301088 H,0,-3.7147909626,-0.5909324258,0.7789782022

POH + X=H, Y=Cl	C,0,-1.5148750171,0.1416404843,0.0610881124 C,0,0.3426927216,-0.9011038564,-0.8377167811 H,0,-0.2700042079,-1.7910285862,-0.9381032809 H,0,0.3148219628,-0.1957203825,-1.6615418534 C,0,1.4228778818,-0.9559488357,-0.0174229257 H,0,1.5975422752,-1.7270831077,0.7216202071 C,0,-1.0712296985,1.5689703621,0.2069946309 H,0,-0.1900149002,1.636673756,0.8494862544 H,0,-0.8055984731,2.0102928925,-0.762108497 H,0,-1.8655010888,2.1922974822,0.6486834849 C,0,-1.7771947993,-0.6601166922,1.2980026414 H,0,-2.6136866506,-0.2393123966,1.8770380672 H,0,-2.0398079676,-1.6907626107,1.0416413083 H,0,-0.8923612075,-0.6713141611,1.9403577342 O,0,-2.4778350582,-0.1003187345,-0.9013016913 H,0,-2.3534550869,0.5232081398,-1.6299599894 Cl,0,2.6192423106,0.3290970634,0.0504485899
POH + X=Me, Y=Cl	C,0,-1.733856666,-0.1093276971,-0.0618764923 C,0,0.212463842,0.196697794,1.1202761068 H,0,-0.2728898014,1.0355981111,1.6089655265 H,0,0.0631175525,-0.777722007,1.5716177729 C,0,1.3307898473,0.4417355782,0.3817360183 C,0,-1.5369456921,-1.442013677,-0.7268593587 H,0,-0.6576615955,-1.4252324099,-1.3752804914 H,0,-1.3851857115,-2.2416036203,0.0094928338 H,0,-2.4103283814,-1.7180228971,-1.3397342825 C,0,-1.8216475,1.1133597342,-0.9223566168 H,0,-2.7193662759,1.088981853,-1.5597691372 H,0,-1.8804776176,2.0165918734,-0.3077574626 H,0,-0.9468749266,1.1862274571,-1.5734305084 O,0,-2.6855584041,-0.0707972154,0.943627422 H,0,-2.6856562385,-0.9212545981,1.4038344397 Cl,0,2.2898710591,-0.9339562273,-0.2048175924 C,0,1.8176320634,1.7718182819,-0.0978105852 H,0,1.1921890703,2.5683583008,0.3155370148 H,0,2.8542395403,1.9499089343,0.2130154322 H,0,1.7949382447,1.848182505,-1.1922658752
POH + X=Cl, Y=Cl	C,0,1.9546300948,-0.000021004,-0.1469697721 C,0,0.0030367992,-0.0000280671,1.1514832365 H,0,0.3660789191,-0.9252943253,1.5806096974

	H,0,0.3661051335,0.9252105714,1.5806464763 C,0,-1.1599601995,0.0000021907,0.4582322273 O,0,2.7929343118,-0.0000434644,0.9631052157 H,0,3.7217606208,0.0001006876,0.6767607678 C,0,1.8942808884,1.2929809081,-0.9043622992 H,0,1.0548370791,1.3068557971,-1.6051224624 H,0,1.7978591147,2.1426679399,-0.2225292605 H,0,2.8155490772,1.4481124205,-1.4934174351 C,0,1.8942537827,-1.2930060314,-0.9043899573 H,0,1.7978376082,-2.1427063257,-0.222573004 H,0,1.0547973385,-1.3068572906,-1.6051356848 H,0,2.8155116077,-1.4481325966,-1.4934613712 Cl,0,-1.9308952395,1.4697854944,-0.0830510911 Cl,0,-1.9309435362,-1.4697370909,-0.0831006772
POH + X=H, Y=CO2Me	
POH + X=Me, Y=CO2Me	C,0,2.1756827056,-0.3528809216,0.1882140426 C,0,0.6100776922,1.0039388627,-1.0770687937 H,0,1.2054776988,1.8995679198,-1.2278865253 H,0,0.8199747515,0.164211556,-1.7256261117 C,0,-0.577204186,1.0833939911,-0.3999480423 C,0,1.7316836578,-0.1161660968,1.6027004024 H,0,0.6622900895,-0.3120638141,1.7245032248 H,0,2.2689644254,-0.7893248905,2.2895101969 H,0,1.9324727518,0.9126479921,1.9136246329 C,0,3.534163384,0.1099282383,-0.2396298416 H,0,4.3180165136,-0.5457722998,0.1728924499 H,0,3.6291759711,0.0784920499,-1.329156925 H,0,3.7343072391,1.1264632503,0.1093883963 O,0,1.8237514264,-1.5337522312,-0.3877792789 H,0,0.8510912013,-1.6514261047,-0.2953868576 C,0,-1.36448757,-0.14535551,-0.2675667405 O,0,-0.9432459015,-1.2954438249,-0.4300911769 O,0,-2.6496589146,0.0852591979,0.0898350304 C,0,-3.4639157424,-1.0814500732,0.2751261744 H,0,-3.5467764378,-1.6475020114,-0.6559726841 H,0,-3.0394730562,-1.7327402299,1.0434011525 H,0,-4.4412771483,-0.7108354647,0.5842122718 C,0,-1.0785642044,2.349939699,0.2475500915 H,0,-0.3501258019,3.1561567319,0.1262977242 H,0,-2.0241573815,2.6758666823,-0.2004962718 H,0,-1.2713481197,2.2196643617,1.3187149729

POH + X=H, Y=CN	C,0,-1.4514337352,0.1977896798,0.0636375543 C,0,0.5200942018,-1.0471871124,-0.8290403526 H,0,-0.1592849153,-1.889870272,-0.8701009339 H,0,0.4802704709,-0.344837579,-1.6537713114 C,0,1.5685918312,-1.0462987583,0.0371306588 H,0,1.6684738868,-1.8185017254,0.7947879479 C,0,-0.8957605485,1.5873567883,0.1238090323 H,0,-0.6405533978,1.9663532933,-0.8738092093 H,0,-1.6172938364,2.2916833581,0.5696496034 H,0,0.0147522783,1.6155502658,0.7280124939 C,0,-1.7108617191,-0.5584520824,1.3255417005 H,0,-2.5115252443,-0.0865897899,1.9171606798 H,0,-2.0260325852,-1.5825247057,1.105764247 H,0,-0.8107012752,-0.5893547002,1.9455231635 O,0,-2.3984628154,-0.0620511357,-0.8978686568 H,0,-2.2752214356,0.5482342317,-1.6381457233 C,0,2.5541846946,-0.0219518132,0.0514321083 N,0,3.3651328897,0.8169609282,0.0746877266
POH + X=H, Y=CHO	
POH + X=Me, Y=CN	C,0,-1.6842567863,-0.1218295782,-0.1006886412 C,0,0.354482099,0.3138150632,1.1529463814 H,0,-0.1614234767,1.1945203389,1.5186914284 H,0,0.1459798751,-0.6203333131,1.6614658249 C,0,1.4691269923,0.4430025019,0.3733017839 C,0,-1.4343000113,-1.5130935081,-0.6008850919 H,0,-1.3260328603,-2.2273175519,0.2250214144 H,0,-2.2624628375,-1.86624611,-1.2367462557 H,0,-0.5159919345,-1.5556913321,-1.1921055996 C,0,-1.7149464801,1.0163090195,-1.0697765156 H,0,-2.5813610987,0.9389954294,-1.7458940498 H,0,-1.7945378641,1.9723976323,-0.544547493 H,0,-0.8108879516,1.0223364789,-1.6836593126 O,0,-2.6358042031,0.0245797133,0.883321704 H,0,-2.6780210993,-0.7882073889,1.4059552793 C,0,2.2223849545,-0.7203617502,0.0299682355 N,0,2.8499508201,-1.6585068238,-0.2675922907 C,0,1.9407770739,1.7567492668,-0.2068178421 H,0,1.2950865662,2.5735377035,0.125186273 H,0,2.9665985516,1.9802252302,0.1078478148 H,0,1.9402249615,1.7411468531,-1.302932781

POH + X=H, Y=Ph	C,0,-2.698350452,0.2221552377,0.2891627187 C,0,-1.1041904275,-0.5538254613,-1.3451274457 H,0,-1.9092177917,-1.1705847865,-1.7308385689 H,0,-1.0883336707,0.4680193626,-1.7085210702 C,0,-0.0077812894,-1.1481788463,-0.7919092323 H,0,-0.0627401273,-2.2151867581,-0.5792810758 C,0,-1.9719447096,1.3435308604,0.9610512956 H,0,-1.7980630181,2.1646580332,0.2597182515 H,0,-2.5535017964,1.7493901546,1.804967612 H,0,-1.0087372692,1.0010914664,1.3474130473 C,0,-2.9709529347,-1.0350892505,1.0598252351 H,0,-3.6760542209,-0.8598112654,1.8889945624 H,0,-3.4021581962,-1.8161086824,0.4200920524 H,0,-2.0439374375,-1.4307664341,1.4830933909 O,0,-3.724812336,0.6910889966,-0.5070153832 H,0,-4.2306425225,-0.0633245823,-0.8387255855 C,0,1.2426159561,-0.5092579424,-0.3958880078 C,0,1.5204742561,0.8578939072,-0.6155398924 C,0,2.7336926888,1.4156180077,-0.2268150144 C,0,3.7119581265,0.6310574342,0.3924049704 C,0,3.4583899898,-0.7237966623,0.615812642 C,0,2.2441157167,-1.2829637868,0.227728537 H,0,0.7788880817,1.4860850831,-1.0990415358 H,0,2.9207150176,2.470366333,-0.4094042199 H,0,4.6580881857,1.0705192258,0.6937670886 H,0,4.209279673,-1.3466865733,1.0941139208 H,0,2.0567522546,-2.3392335353,0.4055403585
POH + X=Me, Y=Ph	C,0,2.215857,-0.260090,0.145828 C,0,0.648246,0.372534 -1.244233 H,0,1.267204,1.114666,-1.744778 H,0,0.603413,-0.602676,-1.719703 C,6,0,-0.495147,0.821677,-0.576780 C,8,0,3.395776,-0.184619,-0.572774 H,0,3.728747,0.724114,-0.554390 C,0,-1.493782,-0.176900,-0.190160 O,0,-1.395976,-1.389026,-0.344950 O,0,-2.595467,0.389909,0.386385 C,0,-3.615319,-0.534790,0.778301 H,0,-4.406381,0.067676,1.226154 H,0,-3.997913,-1.083582,-0.086697 H,0,-3.229733,-1.258181,1.502055

	C,0,-0.706914,2.267112,-0.213469 H,0,-1.651594,2.643581,-0.622236 H,0,-0.765250,2.418540,0.871610 H,0,0.104624,2.889254,-0.601680 C,0,1.876162,-1.703105,0.421447 H,0,1.998181,-2.309258,-0.479929 H,0,2.557988,-2.102911,1.186708 H,0,0.847732,-1.810548,0.769940 C,0,2.133294,0.691144,1.316665 H,0,2.859707,0.398343,2.089031 H,0,2.355342,1.725107,1.024857 H,0,1.138179,0.675128,1.766363
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PEst + X=H, Y=Me	
	C,0,-1.021218256,0.8741652315,-0.1920643911 C,0,-2.0584261534,-1.1277939002,0.0211390809 H,0,-1.3752549462,-1.5181210142,-0.7245287841 H,0,-1.7159479276,-1.1813769376,1.0527569967 C,0,-3.3984004198,-1.0547537794,-0.2403415678 H,0,-3.7357314797,-1.1679131566,-1.2703510864 C,0,-4.4596324954,-0.7698226593,0.7800030838 H,0,-5.2153671093,-1.5670629024,0.8004777133 H,0,-4.0379200944,-0.683366923,1.7863983486 H,0,-5.004882249,0.1596606294,0.5624624993 C,0,-1.2093432891,1.2656977573,-1.630664245 H,0,-0.7372698776,2.2398748575,-1.8345892921 H,0,-0.7848360775,0.5298857023,-2.313141626 H,0,-2.2790762284,1.3644266268,-1.8354981003 C,0,-1.6845111088,1.7296512182,0.847472875 H,0,-1.5448905457,1.3161965696,1.8505362634 H,0,-1.269911073,2.7496771947,0.8468096354 H,0,-2.7558727816,1.8020067185,0.6454286187 O,0,0.3108465024,0.6382883501,0.2269074104 C,0,1.1620658032,-0.2017703003,-0.4209277288 O,0,0.8613648583,-0.8676872403,-1.3892982558 C,0,2.543322102,-0.1979224209,0.2499195433 C,0,3.470063339,-1.1443100827,-0.5283595878 H,0,3.5825648527,-0.8227796305,-1.5671185576 H,0,4.4600559049,-1.1610913924,-0.061340826 H,0,3.0747627231,-2.1631914884,-0.5409130235 C,0,2.391744791,-0.6827169624,1.7094222371 H,0,3.3722747735,-0.6993767726,2.1966868388 H,0,1.7340873568,-0.0229841855,2.2801881377 H,0,1.9806514897,-1.6969528669,1.7486217631

	C,0,3.1120150166,1.2381998913,0.2346032474 H,0,4.1029989721,1.2482432889,0.7007583229 H,0,3.2200804334,1.6108007532,-0.7895403771 H,0,2.465717022,1.9268920919,0.7838080169
PEst + X=Me, Y=Me	C,0,0.7075347209,0.8353060891,0.6604006658 C,0,1.4763272279,2.1200611992,0.4897603725 H,0,2.5371360959,1.9759811949,0.7144745349 H,0,1.3679931006,2.5161612555,-0.5213581332 H,0,1.0980610596,2.8873934634,1.1813150747 C,0,0.8551687758,0.1445686717,1.9925981252 H,0,0.3872173148,-0.8409104491,1.9996064828 H,0,1.911747109,0.0389534398,2.2568199032 H,0,0.38038414,0.7375178226,2.7883450286 C,0,-0.6102598091,0.8181402233,-0.0087937806 O,0,-0.9323896422,1.5975164618,-0.8971224358 O,0,-1.3921466103,-0.2048638647,0.4306707311 C,0,-2.7323402454,-0.4439447181,-0.1252155391 C,0,-3.2128011538,-1.660553568,0.6704081173 H,0,-2.5415443599,-2.5108620783,0.5183425624 H,0,-3.2439815491,-1.4338622245,1.7400237606 H,0,-4.2173276277,-1.9507911011,0.3481458504 C,0,-3.6353336934,0.7660406401,0.140239361 H,0,-3.6455739295,1.0032893818,1.2087913382 H,0,-3.2917323831,1.6399437997,-0.4129506811 H,0,-4.6606732967,0.5331038324,-0.1651810636 C,0,-2.6354726019,-0.7768164945,-1.618383155 H,0,-2.2725124615,0.0793110693,-2.1868787713 H,0,-1.9582279418,-1.6222415535,-1.7767273566 H,0,-3.6234080161,-1.0599682914,-1.9963654374 C,0,1.6469005151,-0.5409677728,-0.7556367248 C,0,2.9898247398,-0.7325268562,-0.4934101118 H,0,1.3594416073,0.0835670064,-1.5968829453 H,0,0.9449312402,-1.3293850411,-0.4985291811 C,0,3.4700100905,-1.8065133255,0.4427409252 H,0,4.1843061926,-2.4730929301,-0.0611391604 H,0,4.0073376842,-1.3842172638,1.3041209061 H,0,2.6478597186,-2.4172526476,0.8244998962 C,0,4.047352754,0.1520584537,-1.0930960768 H,0,4.6217845405,0.6817475161,-0.319534213 H,0,4.7787132934,-0.4433044454,-1.6581076642 H,0,3.6228905656,0.8985822164,-1.7688901672
PEst + X=Me, Y=OMe	C,0,-0.3024310885,0.8808353731,0.760418754

	C,0,-0.5519499829,0.0411849509,1.9871029027 H,0,-1.6255651451,-0.0954455066,2.1490853282 H,0,-0.0841335986,-0.9410890051,1.9125804128 H,0,-0.1448854006,0.5348825402,2.8826772422 C,0,-0.9822148819,2.2244044716,0.7242006274 H,0,-0.8198608971,2.7266834069,-0.2312080926 H,0,-2.0565627261,2.124331498,0.9079789116 H,0,-0.5806198604,2.8822882739,1.509288026 C,0,1.0143519156,0.8390922934,0.1044719921 O,0,1.4118357298,1.6881019478,-0.6872611566 O,0,1.7088648262,-0.2909028527,0.4196111823 C,0,3.0283814082,-0.5702312191,-0.1596619516 C,0,3.3991881202,-1.9109133715,0.4806539159 H,0,3.4317845844,-1.8214121066,1.5703514206 H,0,2.6643567009,-2.6786832769,0.2210243779 H,0,4.3822505483,-2.2398156923,0.1301090932 C,0,2.9226883718,-0.7102099948,-1.6828210967 H,0,2.1761095796,-1.4673690465,-1.9433611184 H,0,2.6418937596,0.2374543998,-2.1419638924 H,0,3.88681076,-1.0312197367,-2.0911979793 C,0,4.0262293491,0.5189069186,0.2510689961 H,0,3.757341888,1.4793805854,-0.1883915899 H,0,4.0482594312,0.6206901687,1.340721896 H,0,5.0315456276,0.2434898026,-0.0845214397 C,0,-1.3245604142,-0.2783721882,-0.8247453425 C,0,-2.6920542151,-0.2820991524,-0.6586799896 H,0,-0.7733265806,-1.172114642,-0.5552993155 H,0,-0.9137785652,0.3268099689,-1.624208276 C,0,-3.6140752075,0.7353768223,-1.2626874714 H,0,-4.4000771268,0.2723525188,-1.8726171187 H,0,-4.1179199235,1.3464141408,-0.5019798772 H,0,-3.0453988075,1.4081927965,-1.9063819067 O,0,-3.191579525,-1.2080944006,0.2229274397 C,0,-4.5930455082,-1.4394001057,0.2741232912 H,0,-4.9761324061,-1.8250969799,-0.6790586222 H,0,-4.7427483899,-2.1958966163,1.0460644209 H,0,-5.1553588998,-0.5391138374,0.5474206112
PEst + X=H, Y=Cl	C,0,-0.6522266237,0.9520183718,0.3788954815 C,0,-0.6889862189,0.933990347,1.8843858898 H,0,-1.7227031495,0.8932504649,2.2408560967 H,0,-0.1326787881,0.0932668172,2.301362751 H,0,-0.2417171023,1.8546097612,2.2863463985 C,0,-1.5380100458,1.9588256267,-0.3032720384 H,0,-1.4853661253,1.8645607854,-1.3888584252

	H,0,-2.5761424117,1.8560310901,0.0237253417 H,0,-1.2138207526,2.9785296229,-0.0470343628 C,0,0.6247231801,0.6686689095,-0.3179731845 O,0,0.8288108262,0.9449930953,-1.4922401191 O,0,1.5051794954,0.0139161723,0.4815762883 C,0,2.8333266152,-0.398641227,-0.0050690775 C,0,3.4498778821,-1.0631819961,1.22829604 H,0,3.5166371677,-0.3527321587,2.0572295236 H,0,2.8445179384,-1.9148850127,1.5522299154 H,0,4.4571239851,-1.4230201966,0.9984359863 C,0,2.6855242313,-1.4080107272,-1.1487103318 H,0,2.0729197819,-2.2577134471,-0.8303728667 H,0,2.2263891446,-0.9462944504,-2.0226990407 H,0,3.6721999143,-1.7911245513,-1.4287728663 C,0,3.6450798576,0.8331625502,-0.4199842347 H,0,3.2065897923,1.3176087631,-1.2923285815 H,0,3.68764996,1.5534517756,0.402962539 H,0,4.6697053645,0.5318127068,-0.6605241796 C,0,-1.5615322228,-0.9831436032,-0.1724341921 C,0,-2.7888643638,-1.1456163923,0.4096281241 H,0,-0.7360577514,-1.5311988321,0.2716313375 H,0,-1.4851556649,-0.7612927792,-1.2314354643 H,0,-2.9413738957,-1.535983673,1.4079709294 Cl,0,-4.2673008075,-0.599328352,-0.3387052497
PEst + X=Me, Y=Cl	C,0,0.3918742121,0.9114857205,0.7562802727 C,0,1.0608799697,2.2600345054,0.7406759911 H,0,2.1343480481,2.1672685615,0.9288157908 H,0,0.8956198704,2.7770766682,-0.2061124319 H,0,0.646861071,2.8980326492,1.5352639355 C,0,0.6258403863,0.0612255795,1.9772744719 H,0,0.2310534465,-0.9485347421,1.8599823998 H,0,1.6929680959,-0.0011382848,2.2080537998 H,0,0.1286415599,0.5084366067,2.851056581 C,0,-0.9292785394,0.8687859838,0.089210242 O,0,-1.3170015459,1.7226111282,-0.6985083465 O,0,-1.6205289948,-0.256088566,0.4031827961 C,0,-2.9492701969,-0.5335596917,-0.1686249308 C,0,-3.3144577859,-1.8750152893,0.4717169547 H,0,-2.5837859769,-2.6434653528,0.2029567241 H,0,-3.3375943413,-1.7886396406,1.5617975466 H,0,-4.3010325735,-2.2009215543,0.1289274504 C,0,-3.9383805042,0.5576873145,0.2547457794 H,0,-3.9517836464,0.65569882,1.3447707236 H,0,-3.672650255,1.51932089,-0.1843706937

	H,0,-4.9468004272,0.2858081924,-0.0735713213 C,0,-2.8522781922,-0.6675270833,-1.6921809679 H,0,-2.5760374621,0.2812477293,-2.151920548 H,0,-2.1088154575,-1.4246561351,-1.9612600458 H,0,-3.8194079293,-0.9869834934,-2.0940019029 C,0,1.4088528331,-0.1955583429,-0.8583106734 C,0,2.770260774,-0.2491457143,-0.6908489979 H,0,1.0313225444,0.4927921634,-1.6087155967 H,0,0.8113681088,-1.0799268809,-0.6697075499 Cl,0,3.4648375163,-1.5693334627,0.2533432486 C,0,3.7656697403,0.7580776645,-1.1685020162 H,0,4.3015487504,1.2272125492,-0.3344208545 H,0,4.5216039674,0.2877235346,-1.8089283258 H,0,3.2623029736,1.5411922084,-1.7414632573
PEst + X=Cl, Y=Cl	C,0,-0.1399910722,-0.8312763104,0.9061790873 C,0,-0.8480557045,-2.1540464004,1.0060648425 H,0,-1.9147327948,-2.0177477272,1.203655723 H,0,-0.7148699422,-2.7473916974,0.1003286549 H,0,-0.4345756312,-2.7380527805,1.8418704021 C,0,-0.321669083,0.1247566168,2.0540754521 H,0,0.0927080662,1.1110726384,1.842314003 H,0,-1.3799187899,0.2292132266,2.3093686755 H,0,0.1905228774,-0.2599496295,2.9486798104 C,0,1.1556019105,-0.8660958594,0.1872063489 O,0,1.4976374273,-1.7884839802,-0.5407122747 O,0,1.8747781372,0.2669347496,0.3828399744 C,0,3.1931709778,0.4661290786,-0.2467429664 C,0,3.6064029135,1.8451087331,0.2730986952 H,0,2.8837444294,2.606912556,-0.0335701546 H,0,3.6642935148,1.844769877,1.3652556318 H,0,4.5874893368,2.1187149435,-0.1260268915 C,0,4.1701209834,-0.6111941977,0.2358694526 H,0,4.2114010958,-0.62368049,1.3295130789 H,0,3.8741252204,-1.5982744474,-0.1192832107 H,0,5.1743273375,-0.3878515212,-0.1384725767 C,0,3.0536395799,0.4806024283,-1.7727023906 H,0,2.7455749127,-0.4947199186,-2.1493094923 H,0,2.31919754,1.2313332677,-2.081837858 H,0,4.0151840202,0.7455156285,-2.224316554 C,0,-1.1862878316,0.1848427325,-0.7894661189 C,0,-2.5117964538,0.4137343315,-0.5405504642 H,0,-0.9253259771,-0.6222810889,-1.4643494535 H,0,-0.5086953073,1.0289385956,-0.7354114245 Cl,0,-3.0730707333,1.8489212663,0.2684031467

	Cl,0,-3.7437876046,-0.7647738842,-0.8850867698
PEst + X=H, Y=CO2Me	C,0,-5.254462728,-1.1644205807,0.3226105856 O,0,-4.4245322199,-0.1656423784,-0.2853548241 C,0,-3.1028612634,-0.4761579564,-0.3500424256 O,0,-2.6426655924,-1.5200257856,0.0837492369 C,0,-2.33970031,0.5921875157,-1.0059237787 C,0,-0.9892513427,0.4645836631,-1.2062762771 C,0,0.1093930939,1.3228515019,0.5584237051 C,0,1.4395774222,0.9470927684,0.0160993456 O,0,1.818795834,-0.2852219597,0.4239000987 C,0,3.0884741287,-0.893530535,-0.0158679331 C,0,4.268441379,-0.0431921287,0.4661251213 O,0,2.0823363609,1.6631522152,-0.7399103268 C,0,3.0700314183,-2.2502071017,0.6919986732 C,0,3.0846832891,-1.0728111276,-1.537352371 C,0,-0.2252507134,2.7858696789,0.4696138101 C,0,-0.455123924,0.5572319516,1.722248917 H,0,-0.4673845589,1.1539662167,-1.860394417 H,0,-0.538157043,-0.5095403575,-1.048064859 H,0,-2.8812715978,1.4867562726,-1.2950714418 H,0,-6.2691461597,-0.76777252,0.2873644068 H,0,-5.1925529247,-2.107082994,-0.2274337653 H,0,-4.9497963503,-1.3448797038,1.3569601185 H,0,3.9739335923,-2.8150765491,0.4451654419 H,0,3.0289108083,-2.1191733566,1.7770613905 H,0,2.1995041552,-2.835808638,0.3831386728 H,0,2.2100941195,-1.6515128949,-1.8507549767 H,0,3.0750808476,-0.1090693093,-2.0466662963 H,0,3.9804357703,-1.623480758,-1.8423543866 H,0,4.2779019889,0.9303324359,-0.024134775 H,0,4.2128189827,0.1040102133,1.549243097 H,0,5.2069913769,-0.5604391189,0.2424187803 H,0,0.1108714176,0.7952727563,2.6350803752 H,0,-1.4962209085,0.8405627731,1.8992322162 H,0,-0.4069158804,-0.521439374,1.5732718283 H,0,0.2143024867,3.3211288672,1.3244620683 H,0,0.1821523418,3.2341770486,-0.4378624682 H,0,-1.3067302228,2.9439863627,0.510321278
PEst + X=Me, Y=CO2Me	C,0,-3.0929004717,0.6980695523,-1.7327450699 C,0,-3.1426333002,0.7644465877,-0.2026204667 C,0,-3.1925927981,2.2173572946,0.2763434636 O,0,-1.8723111318,0.2820118872,0.3681290538

	C,0,-1.4426884745,-0.9887869716,0.1783765284 O,0,-2.0358621266,-1.8331845456,-0.4794615677 C,0,-0.1290002478,-1.231951237,0.8220075733 C,0,1.0187800032,-0.5831426813,-1.009119571 C,0,2.3731678041,-0.6170998293,-0.7616585026 C,0,3.2165326451,-1.8448192133,-0.9608077425 C,0,3.0982522325,0.5659470415,-0.2530618132 O,0,2.3087577718,1.6633084692,-0.095458932 C,0,2.9883532555,2.8336901611,0.3781454931 C,0,-4.3131421004,-0.0386742939,0.3746676377 O,0,4.2930157865,0.5771346252,-0.0070278992 C,0,0.2467893205,-2.6806040726,0.9658823472 C,0,0.3511264135,-0.2934032647,1.8942552508 H,0,0.5606512408,-1.3900651291,-1.5719521526 H,0,0.5065051636,0.3709223916,-1.0219974367 H,0,-2.2275449641,1.2518114691,-2.1106949218 H,0,-3.0341166253,-0.3337293966,-2.07898575 H,0,-3.9952477047,1.1588735056,-2.1476264086 H,0,-4.2780370669,-1.0770245674,0.0448672022 H,0,-4.2889654527,-0.0119607833,1.4685940229 H,0,-5.2585626121,0.4046514356,0.045815654 H,0,-2.3319003542,2.7776935668,-0.1000882091 H,0,-4.1053863467,2.7011270817,-0.0837562106 H,0,-3.1832452466,2.2643034404,1.3690555742 H,0,3.7775663801,3.1315665751,-0.3169957253 H,0,2.2263537909,3.6102896201,0.4459377185 H,0,3.4381778294,2.6519807581,1.3577025705 H,0,2.6234329926,-2.6698161123,-1.3614364664 H,0,4.0441592727,-1.6380488732,-1.6486527843 H,0,3.6823897901,-2.1669586887,-0.022107269 H,0,-0.237265427,-3.1049791439,1.8584121555 H,0,-0.0877339903,-3.2669369859,0.1088149348 H,0,1.3255753967,-2.7980230367,1.0988890381 H,0,-0.2108225407,-0.4680738377,2.8239543733 H,0,1.4074415223,-0.4700317964,2.1170354678 H,0,0.217506864,0.752090579,1.617778614
PEst + X=H, Y=CN	C,0,-3.499357257,0.9458381512,-0.2621582327 C,0,-2.7234473369,-0.3558233023,-0.0371371964 C,0,-3.3421162641,-1.1681333617,1.102652985 O,0,-1.3743219064,-0.0513403638,0.4805368003 C,0,-0.4863752201,0.6792617463,-0.2345977897 O,0,-0.6860314727,1.1160579769,-1.3588969995 C,0,0.7997337681,0.8504787942,0.487549994 C,0,1.6687906184,-1.0683281065,-0.3685773337

	C,0,2.8879950922,-1.3119976217,0.2180619484 C,0,4.1062134892,-0.7891126386,-0.2817435609 N,0,5.1199648099,-0.3678934852,-0.6804306315 C,0,-2.6199892617,-1.1977658929,-1.3129391635 C,0,0.854717331,0.6132852128,1.9709543116 C,0,1.7232703095,1.891651032,-0.0752331041 H,0,0.806351691,-1.6298743947,-0.0276396361 H,0,1.614510368,-0.6483285006,-1.3666842803 H,0,2.9552677946,-1.8800973191,1.1417248449 H,0,-3.5130810069,1.5436060724,0.6545110871 H,0,-3.0545733549,1.5352553978,-1.0639298271 H,0,-4.5346958925,0.711834401,-0.5294693319 H,0,-2.1685626437,-0.6283611879,-2.1253445537 H,0,-2.022030201,-2.0965605708,-1.1309218401 H,0,-3.6208926708,-1.5173332193,-1.6204034966 H,0,-4.3643694616,-1.4592936814,0.8440792625 H,0,-2.7622560663,-2.0763669079,1.2915302679 H,0,-3.3725283664,-0.5802915149,2.0244445412 H,0,1.4657071888,2.8777686343,0.3394401441 H,0,2.7633846267,1.6903591618,0.1965071099 H,0,1.632254074,1.9610956307,-1.1599376285 H,0,0.4185810154,1.4722314351,2.5018541168 H,0,0.2925177365,-0.271953216,2.2711199641 H,0,1.8908769211,0.5176991951,2.3080181216
PEst + X=H, Y=CHO	C,0,-0.6816233069,0.9373141089,0.4248201883 C,0,-0.7455322469,0.8237234576,1.922545669 H,0,-1.7839891212,0.7695387798,2.260967425 H,0,-0.1969175963,-0.041559454,2.2961673422 H,0,-0.298836706,1.7174854102,2.3828066188 C,0,-1.5683278879,1.9615905827,-0.2215636352 H,0,-1.4920948577,1.9264761383,-1.3091826747 H,0,-2.6103932778,1.8314597217,0.0841698781 H,0,-1.2615717237,2.9693206953,0.0954771504 C,0,0.6007157729,0.6746278814,-0.2776706482 O,0,0.8130244994,1.0161798998,-1.4324636274 O,0,1.46755645,-0.0191493867,0.4958000962 C,0,2.8050644012,-0.4088120225,0.0059929892 C,0,3.4022917694,-1.1367118083,1.2122319997 H,0,3.4582321428,-0.4701933206,2.0775631183 H,0,2.7919585465,-2.0032650734,1.4826792333 H,0,4.4122870652,-1.48552923,0.978034128 C,0,2.6698754401,-1.3567656216,-1.1899155926 H,0,2.0528799384,-2.221069467,-0.9241909682 H,0,2.2240374279,-0.8502458578,-2.0458759321

	H,0,3.6599108866,-1.7259646792,-1.4761805759 C,0,3.6208798817,0.8428937947,-0.3328754601 H,0,3.196484739,1.3721123526,-1.1860691087 H,0,3.6518614425,1.5199083278,0.5264358394 H,0,4.6487744908,0.553460005,-0.5735094917 C,0,-1.5889039,-1.0270624801,-0.2574340635 C,0,-2.87632597,-1.1008632481,0.2163150414 H,0,-0.7884588818,-1.5601030207,0.243734141 H,0,-1.4149509742,-0.7745774692,-1.3003642698 H,0,-3.0945276409,-1.4842582546,1.2100234583 C,0,-4.0135890075,-0.6324536881,-0.5636398549 O,0,-5.173426407,-0.6543271353,-0.1730672375 H,0,-3.7590719171,-0.2495083658,-1.5776789601
PESt + X=Me, Y=CN	C,0,-0.5140939174,-0.8071520394,0.8409639156 C,0,-1.2187542289,-2.1315504174,0.9209053409 H,0,-2.2899612234,-1.9974897733,1.0946481446 H,0,-1.0579942428,-2.7257584375,0.0200670336 H,0,-0.8246297651,-2.7138374502,1.7670579939 C,0,-0.7674940914,0.1708688254,1.9540189553 H,0,-0.3115593726,1.1426344516,1.7632878224 H,0,-1.8400552785,0.3067513642,2.1207331624 H,0,-0.3412659441,-0.2135326754,2.8928920578 C,0,0.8130406982,-0.8407982084,0.1790516702 O,0,1.1977741066,-1.7812716873,-0.5031374477 O,0,1.5078796996,0.3034356991,0.3784569988 C,0,2.8507041155,0.507854065,-0.1989157311 C,0,3.2170342762,1.9076473385,0.299158584 H,0,2.4967380851,2.6476319648,-0.0614011658 H,0,3.2252746005,1.9387727425,1.3923337784 H,0,4.2107643038,2.1872218202,-0.0628314364 C,0,3.8211445038,-0.5389825028,0.3575852868 H,0,3.8166285812,-0.5170937163,1.4518042816 H,0,3.5550947972,-1.5411414959,0.0213659889 H,0,4.8368738021,-0.3115436034,0.0184912158 C,0,2.776817412,0.4767034892,-1.7288881822 H,0,2.5021856205,-0.5142873418,-2.0902975613 H,0,2.0440197545,1.2050347984,-2.0906298964 H,0,3.7526105063,0.7457152542,-2.1461050616 C,0,-1.4990682418,0.2054141472,-0.937109109 C,0,-2.8647723026,0.2736713376,-0.7591906481 H,0,-1.0972237703,-0.545691082,-1.6091543799 H,0,-0.8872537539,1.0837352129,-0.7671454678 C,0,-3.4271655208,1.3848571769,-0.0663862733 N,0,-3.9143150924,2.2854456523,0.4946527969

	C,0,-3.8222289396,-0.797991576,-1.2204971146 H,0,-4.3811901958,-1.2288340946,-0.3818605032 H,0,-4.5621426159,-0.3852088548,-1.916156233 H,0,-3.2829212702,-1.6017605598,-1.726405929
PEst + X=H, Y=Ph	C,0,-3.1869363984,-1.0190488275,-0.4710594906 C,0,-2.9900658549,0.3778865957,-0.5610060448 C,0,-4.1206489701,1.2094774335,-0.4034539337 C,0,-5.3831714469,0.6769505134,-0.1630951537 C,0,-5.5552656442,-0.7062852314,-0.0730213234 C,0,-4.4491127779,-1.5484223526,-0.2295063484 C,0,-1.6967192876,0.9868529318,-0.8249160033 C,0,-0.4812247425,0.3534250909,-0.9316329525 C,0,0.5395996824,0.3039204503,1.1145956263 C,0,1.7229901685,-0.4063861292,0.5916724669 O,0,2.6704953038,0.452422536,0.1303343973 C,0,3.9286230963,-0.0306570198,-0.4597814222 C,0,4.6585259689,1.2705357295,-0.8033776261 O,0,1.8131599865,-1.6271385466,0.536093904 C,0,4.7192334233,-0.837101827,0.5765587778 C,0,3.641969823,-0.8422347957,-1.7280224776 C,0,0.6332111009,1.7652539617,1.4586803633 C,0,-0.4013899319,-0.5268576789,1.9393821633 H,0,0.3641040337,0.9050806815,-1.3277089324 H,0,-0.4132237434,-0.726367354,-1.0129720173 H,0,-1.7073185932,2.0729570505,-0.9039569689 H,0,4.8608209245,-0.2472330266,1.4876284826 H,0,4.2020826336,-1.7621261797,0.8310806774 H,0,5.7074611244,-1.0825439337,0.1742040206 H,0,3.0992766958,-1.7577911271,-1.4929978868 H,0,3.052284207,-0.2494083071,-2.4346539107 H,0,4.5862813972,-1.1062546136,-2.215399825 H,0,4.8254578437,1.8683396433,0.0972417106 H,0,5.6287419267,1.0501676554,-1.2585141782 H,0,4.07317977,1.8673475627,-1.5089999428 H,0,-3.9934802408,2.2869719317,-0.4720999282 H,0,-6.2348626284,1.3407173835,-0.0449330025 H,0,-6.5392944581,-1.125201711,0.1145940537 H,0,-4.5746973431,-2.6254668351,-0.1645412012 H,0,-2.3438714948,-1.691129307,-0.5941782936 H,0,-0.0811861431,-0.5271638715,2.9925285468 H,0,-1.41630966,-0.1199916998,1.9104075612 H,0,-0.4126262277,-1.5642250164,1.6018073561 H,0,1.1179371322,1.8960619012,2.437763793 H,0,1.2184374841,2.3259130382,0.7286955569

	H,0,-0.3661462161,2.2052211515,1.5314781909
PEst + X=Me, Y=Ph	C,0,-0.6358026654,0.1564746646,1.1914037992 C,0,-0.7889521382,1.5719982901,1.6786485058 H,0,0.1895842343,2.0245223177,1.8646171289 H,0,-1.3433635863,2.1948484766,0.9754496426 H,0,-1.3380228768,1.5900968217,2.6323520745 C,0,0.3060988823,-0.7242836006,1.962657298 H,0,1.3079296227,-0.2876526098,2.0086386256 H,0,-0.0468508606,-0.8402845623,2.9988652661 H,0,0.3641571386,-1.7216493172,1.5247387529 C,0,-1.7910870398,-0.5309560595,0.5832566208 O,0,-1.8474901085,-1.7424885697,0.4076195519 O,0,-2.7548915042,0.3443866643,0.1899024882 C,0,-3.9899361801,-0.1110964729,-0.466680417 C,0,-4.7454400042,1.1991916994,-0.7043407921 H,0,-4.9383450583,1.7106730199,0.2430702672 H,0,-4.1643099849,1.8691114717,-1.3449197683 H,0,-5.7040873734,0.9993877092,-1.1921803926 C,0,-3.6624968471,-0.7961724236,-1.7981221799 H,0,-3.0677686896,-0.1310984406,-2.432504645 H,0,-3.1091423847,-1.721028741,-1.6363442057 H,0,-4.5916466983,-1.0271406013,-2.3296022205 C,0,-4.7780682524,-1.0270591568,0.4763983617 H,0,-4.2406139137,-1.9576532113,0.6584728168 H,0,-4.953601961,-0.5250523429,1.4330969283 H,0,-5.7512480083,-1.2609884073,0.0325369158 C,0,0.417310691,0.4002526691,-0.8194046242 C,0,1.6498841975,1.0041609339,-0.6669592502 H,0,-0.414075668,0.9963931803,-1.1797855096 H,0,0.3270807508,-0.6654166782,-0.9910156089 C,0,2.8920397257,0.2454544357,-0.4538437883 C,0,2.9393226418,-1.1663094234,-0.5344475605 C,0,4.1259241107,-1.864176117,-0.3464308642 C,0,5.3154779493,-1.1826076808,-0.0714792987 C,0,5.296224128,0.2095576759,0.0102463232 C,0,4.1076298973,0.9109585308,-0.1785141264 H,0,2.0371531498,-1.726169197,-0.7527841895 H,0,4.1245435987,-2.9481078141,-0.4178172369 H,0,6.2417095753,-1.7302603064,0.0740485033 H,0,6.2110820135,0.7555923173,0.2225546048 H,0,4.1258330979,1.9923831328,-0.1070615603 C,0,1.7261815877,2.5131592095,-0.6904805828 H,0,2.0752350233,2.9272146303,0.2641943613 H,0,2.4244544739,2.8661982653,-1.4595557637

	H,0,0.747503183,2.9496130838,-0.9006856534
MEst + X=H, Y=Me	C,0,-1.1917999958,-0.9249673041,-0.97186106 C,0,-2.3744522695,-0.1189778721,0.7996326863 H,0,-1.7002329098,-1.8739374754,-1.080307557 H,0,-1.4239554888,-0.1366326824,-1.6768358221 H,0,-2.0211545854,-0.9464446886,1.4058424891 H,0,-1.7522221788,0.7716376008,0.7967848161 C,0,-3.6865928531,-0.0403918759,0.4320133762 H,0,-4.3232620121,-0.9123317561,0.5784623871 C,0,0.1346878123,-0.9717881473,-0.3721744031 O,0,0.5877437341,-1.9434888687,0.2194603908 O,0,0.7718607111,0.2248832263,-0.508880525 C,0,2.1184681435,0.4430473825,0.0376971526 C,0,2.100071855,0.298824338,1.5636780291 H,0,1.3555544635,0.9721608187,2.0005866122 H,0,1.8677155005,-0.7250701454,1.8566023044 H,0,3.0800740609,0.5692406954,1.9705445271 C,0,3.1165004924,-0.5168908624,-0.6201569258 H,0,2.9052059294,-1.550049326,-0.3443976034 H,0,3.0695598799,-0.4237014333,-1.7096667142 H,0,4.1334513442,-0.2658651746,-0.3011272765 C,0,2.413785647,1.8901336021,-0.3654321499 H,0,3.4061330857,2.1864588622,-0.0124007224 H,0,2.3851720793,2.0008834941,-1.4532516115 H,0,1.6745479513,2.5698990038,0.0684327144 C,0,-4.3097233973,1.1367626233,-0.2504947836 H,0,-3.6082987255,1.9719202029,-0.3374029919 H,0,-4.656750174,0.8773040961,-1.2603397304 H,0,-5.194046388,1.4888617433,0.2964237218
MEst + X=Me, Y=Me	C,0,0.819450703,-0.6693802752,-1.1079705293 C,0,2.0005388149,0.0969499764,0.6930602321 H,0,0.9638093243,0.1841795287,-1.7582520314 H,0,1.3984918092,-1.5632396082,-1.2997285094 H,0,1.3147134381,0.9338959247,0.7784662267 H,0,1.7306772301,-0.799784101,1.2417358864 C,0,3.293046179,0.3013447072,0.2934264056 C,0,-0.4747553607,-0.865858695,-0.4738475977 O,0,-0.8263445196,-1.9071783005,0.0673548545 O,0,-1.2132043826,0.2800907454,-0.5110354736 C,0,-2.5488143864,0.3504447128,0.0944469881

	C,0,-3.4927548363,-0.6453314598,-0.5900095704 H,0,-3.4946653344,-0.4821082142,-1.6723224024 H,0,-3.1906218695,-1.6730063941,-0.3882700001 H,0,-4.5135383728,-0.4969801051,-0.2224976955 C,0,-2.4580119313,0.1124501368,1.6064630077 H,0,-2.1302910051,-0.9044670981,1.8223797281 H,0,-1.7538559018,0.817293424,2.0603849415 H,0,-3.4394949489,0.2734092579,2.0644534755 C,0,-2.9773928929,1.7904899366,-0.200899511 H,0,-3.0036926778,1.9715001515,-1.2793160947 H,0,-3.974730144,1.979436346,0.2075129134 H,0,-2.2780635582,2.500958485,0.2496320531 C,0,4.3158981706,-0.7993769678,0.3394731987 H,0,5.2034059611,-0.4881199464,0.9064593535 H,0,3.9190784404,-1.70863033,0.7981218132 H,0,4.67098327,-1.0532875129,-0.6693648356 C,0,3.7373197468,1.6076749584,-0.3034443858 H,0,2.9398877964,2.3552497765,-0.2941151419 H,0,4.5973186421,2.017602674,0.2428450836 H,0,4.0698338784,1.476356001,-1.3428692394
MEst + X=Me, Y=OMe	C,0,0.3902129179,-0.6363428385,-1.1147640324 C,0,1.5868285394,0.1660878856,0.7188646931 H,0,0.5168299422,0.2188878682,-1.7663876911 H,0,1.0110480929,-1.5074326597,-1.2761458564 H,0,0.8954122096,0.9910966768,0.8269559773 H,0,1.3614947504,-0.7532695511,1.2449392762 C,0,2.8647910971,0.4114315083,0.3067494465 C,0,-0.8902659825,-0.8553634358,-0.4730359145 O,0,-1.2179520832,-1.8947614504,0.0889293326 O,0,-1.6614559521,0.2735667441,-0.5246361922 C,0,-2.995144437,0.3138313526,0.0814151416 C,0,-3.4652923268,1.7377045115,-0.2301987291 H,0,-4.4676102564,1.903847013,0.1762449583 H,0,-2.7859997959,2.4728623601,0.2115528219 H,0,-3.4963813683,1.9053113571,-1.3107222348 C,0,-3.913903153,-0.7156916588,-0.5880976998 H,0,-3.926563488,-0.5628299862,-1.6719244092 H,0,-3.5788250188,-1.731560744,-0.3787928397 H,0,-4.9367809006,-0.5951248733,-0.2159216083 C,0,-2.898478267,0.0975643871,1.5968079461 H,0,-2.5427378158,-0.9072204315,1.8244370954 H,0,-2.2127860041,0.8264738786,2.0411511547 H,0,-3.8836515629,0.2382440151,2.0538856946 C,0,3.3120497322,1.7181453428,-0.2802040938

	H,0,4.1788207082,2.1356838608,0.2452802564 H,0,3.5944750811,1.6131780511,-1.335976561 H,0,2.5008078877,2.4453495832,-0.2209312341 O,0,3.7244223612,-0.6511648836,0.3216375266 C,0,5.1070583525,-0.4467220567,0.061182699 H,0,5.5664281007,-1.4351917434,0.1060562786 H,0,5.2849444506,-0.0186381541,-0.9318512242 H,0,5.5738215436,0.1953402089,0.8183880697
MEst + X=H, Y=Cl	C,0,-0.7620466833,-1.0247443916,-1.006241877 C,0,-1.9458188356,-0.3983624804,0.8669883556 H,0,-1.213454061,-1.9964311446,-1.1578222444 H,0,-1.0834465073,-0.2019514949,-1.6325125353 H,0,-1.510440766,-1.2208060862,1.4247161529 H,0,-1.4063100611,0.5414952845,0.8617455476 C,0,-3.2696698143,-0.4483458791,0.5782049964 H,0,-3.8836251751,-1.3331969637,0.6936033281 C,0,0.5787618014,-1.0160942584,-0.4329753896 O,0,1.1081483164,-1.9948234202,0.0774769077 O,0,1.1239432886,0.2274964397,-0.493876689 C,0,2.468996624,0.505161205,0.0362299896 C,0,2.502677089,0.2501497909,1.5471682889 H,0,1.7250723211,0.8346144527,2.049558976 H,0,2.3535038297,-0.8063523069,1.7706173108 H,0,3.4716237867,0.5621963395,1.9503408587 C,0,3.5112728492,-0.3299450866,-0.7157331006 H,0,3.3783380395,-1.3939140731,-0.5194451547 H,0,3.4316303738,-0.1545441448,-1.7931394872 H,0,4.5163074168,-0.0348303,-0.3972471961 C,0,2.6471929776,1.9948052785,-0.2669172743 H,0,1.8755220827,2.5863787099,0.2341683321 H,0,3.626447278,2.3363823607,0.0814582346 H,0,2.5777424422,2.179796425,-1.3425928294 Cl,0,-4.1237552875,0.8849431597,-0.1489761752
MEst + X=Me, Y=Cl	C,0,0.4775983749,-0.5780057034,-1.1442224423 C,0,1.6576865538,0.1912562817,0.6834356232 H,0,0.5875210542,0.2915166938,-1.7800389207 H,0,1.1040119895,-1.4398855863,-1.3334384761 H,0,0.9230376062,0.9749657176,0.8355523823 H,0,1.4784696015,-0.7583711298,1.1718412549 C,0,2.9028729278,0.5468736012,0.2693810429 C,0,-0.8006835777,-0.8276183272,-0.4926085702 O,0,-1.0983556269,-1.8837496258,0.0502095027

	O,0,-1.5849425818,0.2852800978,-0.5207290251 C,0,-2.9225882159,0.2965273435,0.0901384305 C,0,-3.8231447439,-0.7375841141,-0.5951788239 H,0,-3.8412309214,-0.5673825729,-1.6761945094 H,0,-3.4731140344,-1.751785581,-0.402569069 H,0,-4.8467027498,-0.6395710117,-0.219001142 C,0,-2.8149324367,0.0578357884,1.6005965869 H,0,-2.443408698,-0.9447045387,1.8129149029 H,0,-2.1409473313,0.7913970438,2.0549372921 H,0,-3.8006095111,0.1746356567,2.0627047355 C,0,-3.4120343433,1.7175863356,-0.2003784066 H,0,-4.4159593741,1.8627927007,0.2096587215 H,0,-2.7435256772,2.4561421014,0.251802557 H,0,-3.447609622,1.9005313364,-1.2781334436 Cl,0,4.165891554,-0.6801694055,0.2078479597 C,0,3.3100290364,1.8843465477,-0.2592236096 H,0,2.4800584215,2.5910945726,-0.1759955951 H,0,4.1662818094,2.2818280818,0.2968420076 H,0,3.6111352374,1.820126113,-1.3117808195
MEst + X=Cl, Y=Cl	C,0,0.1732380564,-0.6939466056,-1.1924297521 H,0,0.7416089128,-1.5852137417,-1.4244911184 H,0,0.3598091683,0.2087499611,-1.7606242188 C,0,1.4051378256,-0.0791570538,0.7025018508 C,0,2.6850842322,0.1548702164,0.3244723516 H,0,1.1488052803,-1.0272374263,1.1587831813 H,0,0.7334973448,0.7577755127,0.847356695 Cl,0,3.2135130263,1.7086492681,-0.2489215048 Cl,0,3.875488191,-1.1078181822,0.2400665454 C,0,-1.1155451955,-0.8866258859,-0.5394221345 O,0,-1.4864569037,-1.9530099803,-0.0663970316 O,0,-1.8088762498,0.28072252,-0.4831135545 C,0,-3.1418016023,0.3553323469,0.1385237594 C,0,-3.0476362659,0.0070943207,1.6282120162 H,0,-2.7568360869,-1.0337578622,1.7713200943 H,0,-2.3171198725,0.6535885693,2.1253099041 H,0,-4.0196259096,0.1694822653,2.1050918469 C,0,-4.120547324,-0.556997497,-0.6089010521 H,0,-4.131339397,-0.3089064511,-1.6747890157 H,0,-3.848240392,-1.6060151288,-0.4922088892 H,0,-5.1315711633,-0.4091528962,-0.2158092139 C,0,-3.5187692335,1.8264115635,-0.0522981511 H,0,-2.7933304309,2.4790233191,0.442117124 H,0,-3.5442172427,2.0835132182,-1.115009756 H,0,-4.5067586341,2.0204334513,0.3756190365

MEst + X=H, Y=CO2Me	C,0,0.0111110548,-1.0767443163,-1.0205982079 C,0,-1.1194930763,-0.731743433,1.0043323797 H,0,-0.3748237777,-2.0604597629,-1.2530846384 H,0,-0.4377615649,-0.2094954109,-1.4878896785 H,0,-0.5272535063,-1.5001914036,1.4882283418 H,0,-0.7143927016,0.2737116161,0.9728880878 C,0,-2.4399586262,-0.9307576349,0.7455997158 H,0,-2.9158691395,-1.8956670656,0.8866255793 C,0,-3.2648626068,0.1611168467,0.1983603344 O,0,-2.857324702,1.2651015657,-0.1170362817 O,0,-4.5602026715,-0.2199562236,0.0774577988 C,0,-5.4438289814,0.78197067,-0.4475131441 H,0,-6.429933455,0.3191105807,-0.4786858584 H,0,-5.4542880286,1.6640156262,0.1978825113 H,0,-5.1306128311,1.0860850246,-1.4495616046 C,0,1.381606393,-1.0134887042,-0.5215425279 O,0,2.032732407,-1.9992985359,-0.2012529952 O,0,1.8024106123,0.2722348641,-0.4264399349 C,0,3.1471553831,0.6098190618,0.0712874749 C,0,3.1582472479,2.1380354185,-0.008759128 H,0,4.1190899607,2.5270612898,0.3410469433 H,0,3.0033364768,2.4708644276,-1.0389379721 H,0,2.3645226538,2.5628657133,0.6122819715 C,0,3.303054942,0.1385313246,1.5211143998 H,0,2.5053008002,0.5552061171,2.144250521 H,0,3.2734181372,-0.9493225205,1.5858118422 H,0,4.2606886156,0.4892378149,1.919311555 C,0,4.2124386513,0.0087522677,-0.8520811401 H,0,4.2019696635,-1.0804522012,-0.809116094 H,0,4.0403903587,0.3256464148,-1.8854143034 H,0,5.2024708835,0.3641813723,-0.5486668374
MEst + X=Me, Y=CO2Me	C,0,0.0850565083,-0.8986731363,-1.2299826011 C,0,-1.1365550438,-0.8096536154,0.7908896567 H,0,-0.3186349012,-1.830427812,-1.6033770614 H,0,-0.3153452611,0.036025317,-1.6002570051 H,0,-0.5864456982,-1.6705832194,1.1564700507 H,0,-0.6930668873,0.1652018264,0.9482277316 C,0,-2.4537826384,-0.9323291299,0.4569286425 C,0,1.4285250595,-0.9447772265,-0.6671798649 O,0,2.0339737132,-1.9830373059,-0.4339736067 O,0,1.8862761102,0.3066345906,-0.4025703221 C,0,3.2171649194,0.5303954409,0.1844150253

	C,0,3.2945186821,-0.1089638414,1.5755350618 H,0,2.4849511809,0.2637889492,2.2111565408 H,0,3.2259437317,-1.1951487991,1.5134564338 H,0,4.2450536912,0.1578343565,2.0487520816 C,0,4.3023692717,-0.0018751422,-0.75806693 H,0,4.2492105665,-1.0871789838,-0.8450026857 H,0,4.1911234942,0.4401897355,-1.7530643929 H,0,5.2894440376,0.2734419421,-0.3727631914 C,0,3.2864650241,2.0561725177,0.2852079424 H,0,2.4812261963,2.4378074383,0.9196389449 H,0,4.2434935382,2.3622005078,0.718154408 H,0,3.1907563748,2.5133889141,-0.7037651753 C,0,-3.270204302,0.2526540509,0.09203059 O,0,-4.4651429013,0.2066365181,-0.1385013716 O,0,-2.5511528916,1.4021378874,0.0319994095 C,0,-3.3084173235,2.5766406899,-0.2960129452 H,0,-4.0801357194,2.7609981852,0.4557082649 H,0,-2.5889506413,3.3950812893,-0.3139028469 H,0,-3.7896282509,2.4663220462,-1.2709440362 C,0,-3.1705045733,-2.2505352152,0.3887972405 H,0,-3.5300692774,-2.4524538106,-0.6269974061 H,0,-2.5184327074,-3.0696962144,0.7001524822 H,0,-4.0599392155,-2.2400975451,1.027353081
MEst + X=H, Y=CN	C,0,-0.8801043593,-1.031574431,-1.0565444061 C,0,-2.1202174743,-0.4390927576,0.8739854426 H,0,-1.328286884,-2.0052431669,-1.2051767646 H,0,-1.2119404826,-0.2024889933,-1.6689776559 H,0,-1.6566447623,-1.2739585237,1.3865699042 H,0,-1.5842616778,0.503056358,0.8747390889 C,0,-3.4452371789,-0.490668241,0.5520051549 H,0,-4.010214685,-1.4123977481,0.661022702 C,0,0.4454545919,-1.0043811833,-0.4422896307 O,0,0.9651744935,-1.9802562041,0.0818240799 O,0,0.9772125256,0.2404609312,-0.4953854582 C,0,2.3107918555,0.5361839047,0.0629905576 C,0,2.3125283274,0.2861041423,1.5746357594 H,0,1.5183163161,0.8640336388,2.058094741 H,0,2.1712870141,-0.7712694613,1.7994305721 H,0,3.2688949428,0.6105789072,1.9971205177 C,0,3.3751084344,-0.2919320276,-0.664494028 H,0,3.2529267667,-1.3564123651,-0.4635578165 H,0,3.3139176086,-0.1241796236,-1.7442094071 H,0,4.3701177454,0.017694548,-0.3292319494 C,0,2.4772330651,2.0260396992,-0.2435860926

	H,0,3.4449812947,2.3798154088,0.1238228235 H,0,2.4287839531,2.2056733119,-1.3212102334 H,0,1.6889466431,2.6112165008,0.2385735576 C,0,-4.1486727505,0.617112092,0.0076490812 N,0,-4.7381752876,1.5179280294,-0.4406614404
MEst + X=H, Y=CHO	C,0,-0.8919815878,-1.0204985588,-1.0437461318 C,0,-2.0983301426,-0.4059302411,0.9476988837 H,0,-1.3573921345,-1.9834394323,-1.2066008901 H,0,-1.2622417971,-0.151961933,-1.5732425304 H,0,-1.5828066953,-1.1717985029,1.5163856039 H,0,-1.6032186762,0.5515345484,0.8261792423 C,0,-3.4162211578,-0.5238215803,0.6320787403 H,0,-3.9689344084,-1.4338089857,0.8539466786 C,0,0.4496380126,-1.0244869383,-0.4705275722 O,0,0.9970721493,-2.0309168556,-0.0388305537 O,0,0.9719695694,0.2259841405,-0.4531924588 C,0,2.3165578789,0.4941776134,0.0879070953 C,0,2.3628076125,0.1350331067,1.5767816362 H,0,1.5747258732,0.6652474585,2.1208932116 H,0,2.2389756915,-0.9377734034,1.7257696029 H,0,3.3266422046,0.4403743447,1.9966304632 C,0,3.3682623677,-0.2680061737,-0.7254569399 H,0,3.2643622451,-1.3451477699,-0.5932678218 H,0,3.2716272946,-0.0292046876,-1.7890760008 H,0,4.3695290694,0.0322128199,-0.4001394069 C,0,2.4621365107,2.0042577902,-0.1134916683 H,0,1.6816600541,2.5441408938,0.4302117638 H,0,3.4364530121,2.3406760873,0.2531348456 H,0,2.3824743139,2.2617355468,-1.1733618615 C,0,-4.1345747864,0.5569112451,-0.0588965038 O,0,-3.6010037329,1.571679131,-0.4820875534 H,0,-5.2259281795,0.3974241095,-0.1886636101
MEst + X=Me, Y=CN	C,0,-0.5754196688,-0.728933277,-1.2011812746 C,0,-1.8218404189,-0.1890190796,0.7464533217 H,0,-1.1067329881,-1.6390324118,-1.4473070502 H,0,-0.8072222645,0.1779789714,-1.7453627452 H,0,-1.4476802882,-1.1028942253,1.1947299362 H,0,-1.2095803622,0.6991789815,0.8472815632 C,0,-3.1379641291,-0.0974859863,0.3873720818 C,0,0.7244059506,-0.8817306231,-0.555553438 O,0,1.1362418885,-1.9433747574,-0.1063856301 O,0,1.3714891707,0.307748258,-0.4843658148 C,0,2.7059688975,0.4255135746,0.1306199075

	C,0,2.6359608206,0.0456779613,1.6137879886 H,0,1.8809876615,0.6501751679,2.1266851983 H,0,2.3927155506,-1.0095541191,1.7395008316 H,0,3.6029718082,0.2424109007,2.0877254141 C,0,3.7136425515,-0.4334083779,-0.640889807 H,0,3.4833805636,-1.4944511284,-0.5429277669 H,0,3.707973373,-0.1645766793,-1.70172964 H,0,4.7206927194,-0.254126026,-0.2508884406 C,0,3.0206312702,1.9139256413,-0.0349530353 H,0,2.2734579938,2.5269088023,0.4772758267 H,0,4.003407119,2.1395142793,0.3893712676 H,0,3.026880999,2.1921093541,-1.0925695914 C,0,-3.6559306896,1.1579082696,-0.0588916075 N,0,-4.1036255456,2.1694810266,-0.4268246031 C,0,-4.0851280844,-1.2711467629,0.3699764099 H,0,-4.4441149926,-1.4744162548,-0.6456338994 H,0,-3.591601897,-2.1682240784,0.7506254662 H,0,-4.967963648,-1.0701647662,0.9865641284
MEst + X=H, Y=Ph	C,0,0.5192739655,-0.0760622789,-1.2622635679 C,0,-0.5761870359,-0.9173737388,0.7047469218 H,0,0.5999773761,-1.0180267245,-1.7886910245 H,0,-0.2833285351,0.6018809806,-1.5188667602 H,0,0.2395044528,-1.6177479461,0.8422631409 H,0,-0.430554051,0.0700551929,1.1282273322 C,0,-1.8032776054,-1.3639027815,0.3155378555 H,0,-1.8949434053,-2.4086326575,0.0216464373 C,0,1.6815692364,0.4910114705,-0.6011934861 O,0,1.7182294137,1.6230070135,-0.1320141091 O,0,2.6942584473,-0.4164324978,-0.5309656829 C,0,3.9757853603,-0.0887820178,0.1091338134 C,0,4.6531116573,1.0702148838,-0.631335057 H,0,4.7505867752,0.834511652,-1.6957191651 H,0,4.0804907634,1.9915724606,-0.5242764684 H,0,5.6574970696,1.2286731153,-0.2251791327 C,0,3.7608581748,0.2227792492,1.5947903938 H,0,3.1735288449,1.1320778201,1.7224722344 H,0,3.243752635,-0.607609151,2.0863211261 H,0,4.7302108339,0.3554640644,2.0862718961 C,0,4.7768196569,-1.3821430246,-0.0621203673 H,0,4.8920460776,-1.6266936479,-1.1219442229 H,0,5.7720219993,-1.271980093,0.3790239102 H,0,4.2704107915,-2.2176164455,0.4300618563 C,0,-3.026293648,-0.5779124367,0.1964290476 C,0,-4.2210860257,-1.2245151341,-0.1785827674

	C,0,-5.414920254,-0.5194327403,-0.30252296 C,0,-5.4436741229,0.8550704675,-0.0594855556 C,0,-4.2666719801,1.5153916862,0.3077656952 C,0,-3.0739049849,0.8120743734,0.4345849429 H,0,-4.203481876,-2.2944344971,-0.3702194064 H,0,-6.3228195109,-1.0413315504,-0.5906218128 H,0,-6.3725569645,1.4088693801,-0.157377082 H,0,-4.2804923536,2.5854338587,0.4935849263 H,0,-2.1701681768,1.3444301958,0.7139510974
MEst + X=Me, Y=Ph	C,0,0.7079778264,1.516359444,-1.188725224 C,0,-0.6197865545,1.5930590008,0.8112259801 H,0,0.0976607659,0.7674247913,-1.6754187629 H,0,0.5881175456,2.554064347,-1.4700865334 H,0,-0.0737886804,0.7280591239,1.1660026635 H,0,-0.1896216932,2.5581854339,1.0539465943 C,0,-1.9248504352,1.4989779896,0.4134545332 C,0,1.9758788181,1.1408313151,-0.5908008184 O,0,2.8438276529,1.9369449761,-0.2551089807 O,0,2.0505405495,-0.2121059441,-0.4154488467 C,0,3.248123034,-0.8456823145,0.1543312395 C,0,4.4634866514,-0.5697273419,-0.7386659492 H,0,4.2570229548,-0.8822931477,-1.7671014755 H,0,4.7190758278,0.4899037256,-0.7354597507 H,0,5.3234669645,-1.1420090032,-0.3758038094 C,0,3.4692204638,-0.3659796361,1.5935902969 H,0,3.709432708,0.6968534942,1.6192656543 H,0,2.5721875279,-0.5434461571,2.1957754344 H,0,4.2942091851,-0.9266706191,2.0452917486 C,0,2.8884384696,-2.3336197747,0.1299229655 H,0,3.7161241425,-2.9281338862,0.528277231 H,0,2.0005567915,-2.5274360965,0.7391525879 H,0,2.6843715997,-2.6643296356,-0.8925083425 C,0,-2.717383473,2.7586891517,0.1598662739 H,0,-3.5408113453,2.8660723818,0.8771713772 H,0,-2.084167988,3.6436214822,0.2552465271 H,0,-3.1662422078,2.761995677,-0.8403941441 C,0,-2.578561897,0.1956127769,0.1857398607 C,0,-1.8283553726,-0.9916032069,0.0361342222 C,0,-2.4550880417,-2.2159729086,-0.1715614458 C,0,-3.8483637301,-2.2970732116,-0.2408631297 C,0,-4.6068843839,-1.1340158429,-0.1079210443 C,0,-3.9815357524,0.0943987091,0.0954131884 H,0,-0.7442381171,-0.9525905514,0.0541008074 H,0,-1.852066617,-3.1116381034,-0.290346701

	H,0,-4.3348081202,-3.2540420783,-0.4045049017 H,0,-5.6906888415,-1.180823795,-0.1637278262 H,0,-4.594631759,0.9829954609,0.1987385468
PCN + X=H, Y=Me	C,0,-1.0743373293,-0.0895612063,0.0774689397 C,0,0.7166098926,-1.0639077315,-0.7359062826 H,0,0.2064816351,-2.0233870202,-0.7347343618 H,0,0.6490565637,-0.4997219404,-1.6627287901 C,0,1.8144472971,-0.8858087234,0.0742849803 H,0,1.9794901871,-1.5890955838,0.8898606177 C,0,2.7483503087,0.2794182289,-0.0104745921 H,0,2.5335671087,0.9082687469,-0.8782627086 H,0,2.6777198944,0.915243324,0.8825903003 H,0,3.7924819256,-0.0553335087,-0.0720735524 C,0,-1.2185529155,-0.703205461,1.4536307103 H,0,-2.1209171917,-0.3292511942,1.9564783298 H,0,-1.310340536,-1.7915726816,1.3767436736 H,0,-0.3602931644,-0.4713806628,2.088573177 C,0,-0.6701518334,1.2777021844,0.0490381977 N,0,-0.2969617346,2.3839518298,0.0065546736 C,0,-2.1149745915,-0.4809953703,-0.9513415515 H,0,-1.8789650408,-0.0828895379,-1.9417799531 H,0,-2.192034564,-1.5707895503,-1.0225530184 H,0,-3.1058596475,-0.0996047238,-0.6681988402
PCN + X=Me, Y=Me	C,0,1.142386718,0.0037248931,0.4150437311 C,0,-0.4846251923,-0.0061995654,-1.0508201156 H,0,-0.1206827097,0.9069590924,-1.5130845468 H,0,-0.1197961335,-0.9244559517,-1.5021576634 C,0,-1.7302612674,-0.0032743202,-0.451740163 C,0,0.9450480915,-1.2748519691,1.2018051433 H,0,1.0141775864,-2.1599558719,0.5640825828 H,0,1.7077402949,-1.3708740229,1.9870719905 H,0,-0.0337365412,-1.2716387001,1.6898847448 C,0,0.9482148745,1.2955333184,1.1807227686 H,0,1.7110028076,1.4023913243,1.9644887032 H,0,1.0198239587,2.1699111055,0.5286468467 H,0,-0.0306717584,1.3029233671,1.6685699546 C,0,2.2335849585,-0.0051828302,-0.5027712007 N,0,3.0836291188,-0.0128877136,-1.3048299184 C,0,-2.4352225416,-1.2788477023,-0.0817595507 H,0,-3.4237723147,-1.3288872425,-0.5594992748

	H,0,-1.8698079175,-2.1646417676,-0.3821019427 H,0,-2.6198515123,-1.3428104183,1.0002208095 C,0,-2.4362310262,1.2759031267,-0.0964101498 H,0,-1.8716306239,2.1586344897,-0.4071247004 H,0,-3.424943674,1.3195731734,-0.5744278275 H,0,-2.6206229845,1.3522557112,0.9848169727
PCN + X=Me, Y=OMe	C,0,1.5134752805,0.2383847481,0.3787865416 C,0,-0.0609824953,-0.4380349866,-1.0321160864 H,0,0.176308494,0.3736735671,-1.7099721574 H,0,0.415625426,-1.3891630863,-1.2353737487 C,0,-1.3057547501,-0.4484647653,-0.4421308818 C,0,1.3161914468,-0.6239301208,1.6067989328 H,0,1.4577386164,-1.6857459284,1.3875062384 H,0,2.0290380579,-0.351035621,2.3976970601 H,0,0.3090603756,-0.4814466385,2.0107934109 C,0,1.1954999719,1.7104028533,0.5370321804 H,0,1.8405429922,2.1712120925,1.298865652 H,0,1.3420462492,2.2586985449,-0.3970728131 H,0,0.1558199865,1.8409290996,0.8512207794 C,0,2.6491350277,-0.0757047719,-0.4181227784 N,0,3.5389660475,-0.3617802268,-1.1214652275 C,0,-1.9031052026,-1.6407077457,0.2455254909 H,0,-2.8792297029,-1.913361091,-0.1745121172 H,0,-1.2411789736,-2.50079439,0.1325772315 H,0,-2.0536853201,-1.4708286535,1.3199246695 O,0,-1.9535412809,0.759609247,-0.3819629678 C,0,-3.3370329525,0.7961430559,-0.0527451569 H,0,-3.9430380865,0.259982502,-0.7935415903 H,0,-3.5399385954,0.384714045,0.9425407098 H,0,-3.6180995623,1.850223566,-0.0628624435
PCN + X=H, Y=Cl	C,0,-1.1889934491,0.4280872307,0.0416564661 C,0,0.3372019277,-1.1605932514,0.1796230984 H,0,-0.2784071683,-1.7584812935,0.8443847608 H,0,0.2607232048,-1.3888154494,-0.8777901173 C,0,1.5113563566,-0.6771943965,0.6913173161 H,0,1.7299235059,-0.6072981249,1.7495562318 C,0,-0.6893657947,1.3032077304,-1.0870385881 H,0,0.3085680504,1.6871905224,-0.8595394028 H,0,-0.6487473043,0.7628714314,-2.0359329809 H,0,-1.3566608524,2.1656588606,-1.2229750067 C,0,-1.1891268764,1.0406462616,1.4247470473 H,0,-1.9014216683,1.8752698297,1.4740451819

	H,0,-1.4731538069,0.3164429197,2.1926636027 H,0,-0.1967401896,1.435086081,1.6615237302 C,0,-2.2983786938,-0.4115531151,-0.2661146071 N,0,-3.1691129326,-1.1505632763,-0.5137790849 Cl,0,2.755502702,0.0253185528,-0.3079192236
PCN + X=Me, Y=Cl	C,0,1.4218195226,-0.1569260999,0.4001981121 C,0,-0.1920449996,0.3073773426,-1.0297591141 H,0,0.3050810166,1.2067265384,-1.3800077722 H,0,0.0083853686,-0.5956539376,-1.5943276551 C,0,-1.4098792202,0.4690093471,-0.4149051271 C,0,1.1431761591,-1.5901542301,0.7990287421 H,0,0.1478749791,-1.675565265,1.2431255335 H,0,1.2037476133,-2.2703961629,-0.0540707225 H,0,1.8742611352,-1.9283714436,1.5466465089 C,0,1.2703736353,0.8863352197,1.4856180823 H,0,2.0365317451,0.7498721284,2.2611434159 H,0,1.3739520088,1.9016112864,1.0940605923 H,0,0.2930628755,0.7917044419,1.9672991134 C,0,2.5155730494,0.0379667258,-0.4927822015 N,0,3.3685342271,0.2165542659,-1.2714097492 Cl,0,-2.4200319286,-0.9486192872,-0.1303122226 C,0,-1.9692804774,1.7454239596,0.1257102566 H,0,-1.2902928018,2.574995451,-0.0884863647 H,0,-2.9424286468,1.9667813743,-0.3285623919 H,0,-2.127798112,1.6947500217,1.209703268
PCN + X=Cl, Y=Cl	C,0,-1.6504071637,0.0021540171,0.4417721142 C,0,-0.0004138797,-0.000198092,-1.0624340589 H,0,-0.3531445674,-0.9232773855,-1.5071293713 H,0,-0.3518285283,0.9229314305,-1.5080649303 C,0,1.2411110145,-0.0008229279,-0.4839202319 C,0,-1.4399918598,1.2933272981,1.1999406567 H,0,-0.4587421257,1.2985034932,1.6817142458 H,0,-1.5160608038,2.1681297285,0.5496159242 H,0,-2.1981053508,1.3981947842,1.9885874556 C,0,-1.4362589254,-1.2833113662,1.2084999879 H,0,-1.5092990842,-2.1626075668,0.5639191124 H,0,-0.4551793598,-1.2822318451,1.6906444359 H,0,-2.1943306527,-1.3853366872,1.9975630307 C,0,-2.7179080165,-0.0025063349,-0.5009075884 N,0,-3.5482247474,-0.006429781,-1.3233418267 Cl,0,2.0568147736,1.4659938386,-0.0302549941 Cl,0,2.0548015021,-1.4684146063,-0.0292251467

PCN + X=H, Y=CO₂Me	C,0,-3.970338,-0.016253,0.442288 O,0,-2.853314, 0.572696,-0.239540 C,0,-1.736454,-0.198889,-0.291002 O,0,-1.671983,-1.315038,0.198580 C,0,-0.670148,0.460719,-1.050552 C,0,0.538839,-0.172408,-1.260762 C,0,1.847257,0.274449,0.392557 C,0,2.958093,-0.482611,-0.085670 N,0,3.845179,-1.111198,-0.511370 C,0,1.995037,1.778666,0.310887 C,0,1.124843,-0.287455,1.596909 H,0,1.234643,0.233224,-1.988030 H,0,0.591240,-1.245362,-1.099456 H,0,-0.851140,1.476675,-1.385920 H,0,-4.271047,-0.949005,-0.041619 H,0,-3.719100,-0.229648,1.484635 H,0,-4.772231,0.719566,0.385654 H,0,2.706729,2.135243,1.067563 H,0,2.363750,2.100730,-0.666320 H,0,1.030908,2.258198,0.500878 H,0,1.763382,-0.218602,2.488305 H,0,0.210152,0.280770,1.788147 H,0,0.846893,-1.333540,1.457186
PCN + X=Me, Y=CO₂Me	C,0,-3.8633604515,-0.7873744887,0.3299433181 O,0,-2.8438640142,0.2016484102,0.1227244833 C,0,-1.6658785024,-0.2750033401,-0.3545937154 O,0,-1.4778474862,-1.4589727402,-0.5831075533 C,0,-0.6755938222,0.8070783829,-0.55951933 C,0,-1.021775217,2.2142937683,-0.1594027558 C,0,0.5360188136,0.451937805,-1.1095909197 C,0,2.0030498772,-0.0995587805,0.5104278143 C,0,3.0234835987,-0.5719673783,-0.3622691713 N,0,3.8350836842,-0.9408642393,-1.1179388782 C,0,2.2845576033,1.2181558198,1.1976054883 C,0,1.2653507008,-1.1483145459,1.3087270213 H,0,1.2057647612,1.2239542731,-1.4730232076 H,0,0.6334952424,-0.5310616072,-1.5547225642 H,0,-4.1025058411,-1.2972797575,-0.6065619904 H,0,-3.5358126654,-1.5327041829,1.0591841735 H,0,-4.7309644327,-0.2428568754,0.7021889384 H,0,-0.1975945426,2.8974491223,-0.3784677501 H,0,-1.9122622854,2.5640144636,-0.6939197514

	H,0,-1.2624310544,2.2872766049,0.9077716286 H,0,1.9232973486,-1.5661715841,2.0835403914 H,0,0.403158553,-0.7010244009,1.8107175132 H,0,0.9088119614,-1.9666579503,0.6809641818 H,0,2.9817092095,1.0683275836,2.0340840191 H,0,2.7354199235,1.9471026865,0.5196545304 H,0,1.362904432,1.6387924853,1.6092600955
PCN + X=H, Y=CN	C,0,1.0540531187,0.443246746,0.103734587 C,0,2.1722003662,-0.2895529761,-0.3820245712 N,0,3.0582257702,-0.9383505782,-0.7821937435 C,0,-0.4177582306,-1.2674634006,-0.0000288153 C,0,-1.5890474672,-0.884627033,0.6142430903 C,0,-2.6252771003,-0.1968431762,-0.0634604054 N,0,-3.484212498,0.3753579246,-0.6101998132 C,0,0.4455308979,1.4517136656,-0.8419663616 C,0,1.0736297836,0.7969024396,1.572562205 H,0,-0.350508316,-1.2766952141,-1.0820524623 H,0,0.2561296309,-1.9325710614,0.5276568057 H,0,-1.7367807093,-1.0467868597,1.6782860772 H,0,1.7527411561,1.6428423017,1.7456181239 H,0,0.0763258408,1.0990150142,1.9039435437 H,0,1.4180475761,-0.0357342552,2.1907686886 H,0,1.0435494868,2.3736540583,-0.8399429696 H,0,0.4102688198,1.0824819996,-1.8694241194 H,0,-0.5678546012,1.7144849999,-0.5264571635
PCN + X=H, Y=CHO	C,0,-1.1809944167,0.4562838044,-0.0345021453 C,0,0.3208096716,-1.1509933374,0.4677084041 H,0,-0.2983950317,-1.4816549245,1.2941131163 H,0,0.1533254765,-1.6616670341,-0.4771033041 C,0,-0.6189052506,1.0765130062,-1.2911741803 H,0,0.3782169655,1.4842132056,-1.1029292407 H,0,-0.5608265183,0.3590547073,-2.1130146628 H,0,-1.2605765283,1.906090255,-1.6185320361 C,0,-1.184891955,1.3093457992,1.2129223992 H,0,-1.8797276245,2.1512489687,1.0891902215 H,0,-1.5010663716,0.7463191156,2.0942953155 H,0,-0.1888908898,1.7228898761,1.3925106986 C,0,-2.2902924773,-0.418167792,-0.2046708011 N,0,-3.1708843867,-1.1757771748,-0.332837733 C,0,1.5344984455,-0.5484689209,0.7036284976 H,0,1.7962641927,-0.1650120358,1.6866603279 C,0,2.5174061308,-0.350239063,-0.3538115291

	O,0,3.5930428431,0.2107244825,-0.196142975 H,0,2.2277434018,-0.7624787502,-1.3467863752
PCN + X=Me, Y=CN	C,0,-1.3069864875,0.2633254773,0.3864531013 C,0,0.2862265311,-0.391377144,-1.0754855786 H,0,-0.2556051742,-1.2891755194,-1.3528041746 H,0,0.0879629496,0.4902379441,-1.673656912 C,0,-1.0134559383,1.7387664005,0.536296269 H,0,0.0141904366,1.8954892719,0.8766238368 H,0,-1.1618813282,2.2838026851,-0.3987293376 H,0,-1.6824957562,2.1797686304,1.2883421787 C,0,-1.0766993895,-0.6052410382,1.6010964374 H,0,-1.8025051463,-0.3546539017,2.3869853251 H,0,-1.1884128427,-1.6683042514,1.3745442785 H,0,-0.0772489968,-0.4300010681,2.0083417514 C,0,-2.4193471626,-0.0827989432,-0.4300161082 N,0,-3.2954121166,-0.3906365391,-1.1399451628 C,0,1.4974315654,-0.523072838,-0.4253039597 C,0,1.9894988571,-1.8198841666,0.1689215765 H,0,1.2728065073,-2.6233033821,-0.0157267183 H,0,2.9505626627,-2.1071989031,-0.2729952167 H,0,2.1496507187,-1.736629086,1.2499386323 C,0,2.3230867753,0.6243641129,-0.2469511418 N,0,3.0117617542,1.5528474556,-0.0830444399
PCN + X=H, Y=Ph	C,0,-1.6212352092,-1.0230978407,-0.4140772741 C,0,-1.3831064829,0.3673360785,-0.5033244509 C,0,-2.4300359042,1.2366147312,-0.1257009273 C,0,-3.6515808416,0.7453490687,0.3235071632 C,0,-3.8643866345,-0.6324615676,0.4093936683 C,0,-2.8417636677,-1.5114834213,0.0368263357 C,0,-0.1321961437,0.9346409471,-0.9798233797 C,0,1.0163274572,0.2590368235,-1.320649807 C,0,2.3832885328,0.1097137197,0.5050578361 C,0,3.4307546734,-0.6034978105,-0.135762911 N,0,4.2607102791,-1.1911227304,-0.7138679669 C,0,1.5498043691,-0.662619119,1.4995208301 C,0,2.6539668365,1.5619812125,0.8243390079 H,0,1.7978793772,0.7858257202,-1.8562624685 H,0,1.017361447,-0.8179183125,-1.4515599685 H,0,0.5920372765,-0.1607259207,1.6635090734 H,0,1.3557235721,-1.684440867,1.1647551968 H,0,2.0662281423,-0.722330851,2.4683424068 H,0,3.2840100232,1.6486608538,1.7207586365

	H,0,3.1704476991,2.0713291964,0.0068104598 H,0,1.7148852978,2.0850713528,1.0280350582 H,0,-2.2710346016,2.3100211239,-0.1907688904 H,0,-4.4394388114,1.4369420137,0.6074836328 H,0,-4.8166846075,-1.0189743375,0.7595118456 H,0,-3.0012651883,-2.5842996478,0.0956899999 H,0,-0.8447317047,-1.7226938507,-0.7060596034 H,0,-0.1094117861,2.0223157062,-1.0290061579
PCN + X=Me, Y=Ph	C,0,2.3681075237,-0.1868280657,0.5656301381 C,0,1.0056439338,0.3828279793,-1.1714984194 H,0,1.800975706,0.9766027386,-1.6087693883 H,0,0.9815470826,-0.6492174687,-1.4981507575 C,0,1.4640846549,-0.9807006485,1.4790214686 H,0,0.5974669353,-0.3812661557,1.7720502597 H,0,1.1046628962,-1.896887645,1.0050824822 H,0,1.9989798391,-1.2664588519,2.3961811326 C,0,2.8570048303,1.1462203443,1.0862287983 H,0,3.5303638392,1.0013621039,1.9431803998 H,0,3.4075775853,1.7064203965,0.326239268 H,0,2.015297666,1.7534936114,1.4308308382 C,0,3.2977184231,-0.933398239,-0.2079015581 N,0,4.0278899943,-1.5356856882,-0.8949240456 C,0,-0.1331598672,1.0201507732,-0.7181692206 C,0,-0.1010081947,2.5184570913,-0.5263673774 H,0,0.8433009561,2.9369732855,-0.8808447433 H,0,-0.9139819949,3.0077979863,-1.0763379638 H,0,-0.2172985167,2.8065188047,0.526650815 C,0,-1.3678845852,0.2974601977,-0.3737465678 C,0,-2.4380356423,0.9599399689,0.2679395859 C,0,-3.6157804833,0.2926598863,0.5966113575 C,0,-3.7696776379,-1.0597538438,0.2924266753 C,0,-2.7281923857,-1.7355976973,-0.3505706275 C,0,-1.5525668481,-1.0716070172,-0.6787916882 H,0,-2.3483829901,2.0103923363,0.520025278 H,0,-4.4160556595,0.8338785736,1.0931963537 H,0,-4.6879520229,-1.5802844291,0.5466858203 H,0,-2.8365939825,-2.7863818944,-0.6035027874 H,0,-0.7726596277,-1.6221279518,-1.1929240758
MCN + X=H, Y=Me	C,0,-0.9341926487,0.7525005933,0.4596681629 C,0,0.5617756826,-0.8597569912,-0.0142197546

	H,0,-0.7917412231,0.8008751166,1.5334627842 H,0,-0.4912142774,1.5580524507,-0.1154567242 H,0,0.0096622487,-1.5784525378,0.5819363412 H,0,0.2959455338,-0.8202269319,-1.0667375133 C,0,1.7924034842,-0.4237754553,0.3974426002 H,0,2.1006108915,-0.6229180415,1.4232984443 C,0,-2.1564020137,0.2303165929,-0.0029802991 N,0,-3.1406861935,-0.2578590198,-0.4069093013 C,0,2.7230453769,0.4010934892,-0.4340904714 H,0,2.3451051981,0.537475061,-1.4516700051 H,0,2.8827618489,1.3948722464,0.0071554796 H,0,3.713893846,-0.0669335972,-0.4985451251
MCN + X=Me, Y=Me	C,0,1.2918054321,0.0002530257,0.8623046209 C,0,-0.2118579792,-0.0001135425,-0.8219582508 H,0,0.9889167074,0.920063872,1.350309177 H,0,0.988873015,-0.9192649597,1.3508318537 H,0,0.2056885443,0.9181255461,-1.2224234046 H,0,0.2056921269,-0.9184616028,-1.2221710477 C,0,-1.4652857884,-0.0000399749,-0.2635237213 C,0,2.5389382799,0.0000326917,0.2116360614 N,0,3.5455088884,-0.0002120858,-0.3864766441 C,0,-2.1634480373,-1.2788378393,0.105436401 H,0,-3.1591147999,-1.3288064347,-0.3547750732 H,0,-1.5992460357,-2.1609567615,-0.208285179 H,0,-2.3257828051,-1.3446324632,1.1907770311 C,0,-2.1634162291,1.2788539549,0.105163299 H,0,-1.5992974362,2.1608913705,-0.2089381784 H,0,-3.1591765247,1.3286542094,-0.3548583554 H,0,-2.3255290791,1.3449819317,1.1905192244
MCN + X=Me, Y=OMe	C,0,1.7174321425,-0.1970043738,0.8538127392 C,0,0.2724388331,0.2788987207,-0.8675154316 H,0,1.4831609709,0.6312426971,1.5133823876 H,0,1.2740178781,-1.1535429417,1.1059074209 H,0,0.7791784685,1.2025563981,-1.1134557892 H,0,0.5941628102,-0.6151779436,-1.3866330244 C,0,-0.9909814639,0.3275543525,-0.3428045798 C,0,2.9871937062,-0.2018087152,0.254824156 N,0,4.0196873287,-0.1876508191,-0.2991397918 C,0,-1.6163550993,1.5749968696,0.2080598372 H,0,-0.966913048,2.4300961509,0.0143865372 H,0,-2.592102042,1.7849183979,-0.2451706052 H,0,-1.7729378153,1.5078077717,1.2929499137

	O,0,-1.6300356565,-0.8711380616,-0.196025466 C,0,-3.0039434183,-0.8997864226,0.1733713309 H,0,-3.182694364,-0.4269514472,1.1455410183 H,0,-3.6370462158,-0.4201136046,-0.5828625775 H,0,-3.2710608925,-1.9552778385,0.239648678
MCN + X=H, Y=Cl	C,0,1.3516064148,-0.5824892505,0.6615500194 C,0,-0.0763904652,0.9440828402,-0.2229221621 H,0,1.2432328618,-0.3242467714,1.7089922375 H,0,0.8160794887,-1.4627071808,0.3233942058 H,0,0.5302877833,1.7788783722,0.1114876629 H,0,0.1238593915,0.5613643167,-1.2167415785 C,0,-1.2919331441,0.7623553743,0.3604764438 H,0,-1.6050956994,1.2491430383,1.2761575607 C,0,2.5791266475,-0.2856302306,0.0451819767 N,0,3.573286612,0.0107123435,-0.4975733384 Cl,0,-2.4409309899,-0.4063135635,-0.2227055521
MCN + X=Me, Y=Cl	C,0,-1.5935953215,-0.0799399224,0.8593984051 C,0,-0.1215844502,0.2560632588,-0.84160057 H,0,-1.1694279171,-1.0158610841,1.2056985057 H,0,-1.36987358,0.8002274033,1.4519867038 H,0,-0.4244958342,-0.6786233202,-1.2962849827 H,0,-0.6375933774,1.1501553371,-1.1750231565 C,0,1.1197498488,0.3944575104,-0.2934194016 C,0,-2.8425035369,-0.1250570079,0.2172900782 N,0,-3.8538621902,-0.1492188475,-0.3723996318 C,0,1.7399347405,1.6694541221,0.1782573012 H,0,2.7246148197,1.8178863315,-0.2785600056 H,0,1.1027799487,2.5186487674,-0.082679408 H,0,1.8880171205,1.6621889567,1.2650683821 Cl,0,2.0618239098,-1.0529387191,0.0468845004
MCN + X=Cl, Y=Cl	C,0,-1.8197921478,-0.0000009303,-0.8803821575 C,0,-0.3370775943,-0.0000010878,0.8817763973 H,0,-1.4800397518,0.9240184957,-1.3348393145 H,0,-1.4800406471,-0.9240212267,-1.3348381701 H,0,-0.7457534901,0.9263886345,1.2657005853 H,0,-0.7457521948,-0.9263915413,1.265699825 C,0,0.9181938266,-0.0000001195,0.3575632502 C,0,-3.0726068763,0.0000008147,-0.2484928477 N,0,-4.0901390263,0.0000010282,0.3314539777 Cl,0,1.7338322186,-1.4673792056,-0.0836667329

	Cl,0,1.7338299001,1.4673795805,-0.083667892
MCN + X=H, Y=CO2Me	C,0,2.0362448643,-0.3975515014,0.7835007966 C,0,0.8726866415,0.9846841276,-0.6272610944 H,0,1.8522655728,0.1151106359,1.7206617189 H,0,1.4042274997,-1.2469573468,0.5496146944 H,0,1.6045720594,1.7837298954,-0.5944031865 H,0,1.0042369666,0.2231188412,-1.3877404029 C,0,-0.3521868967,1.1374660089,-0.0428881777 H,0,-0.5870995963,1.986444825,0.5907981385 C,0,3.3434009307,-0.3736596693,0.274496893 N,0,4.4196740947,-0.3141043514,-0.183580869 C,0,-1.3759893292,0.0892173278,-0.1915730752 O,0,-1.1937495714,-0.9969623699,-0.7154424142 O,0,-2.5565498554,0.4732235182,0.346417868 C,0,-3.6168700327,-0.4912196045,0.248580881 H,0,-3.8314652051,-0.7221918297,-0.7977334856 H,0,-3.3447439519,-1.4162063148,0.7631348518 H,0,-4.4810336611,-0.0280275669,0.7237927848
MCN + X=Me, Y=CO2Me	C,0,2.1252364964,-0.387058734,0.8468205049 C,0,0.9101121038,0.5224986605,-0.8984181962 H,0,1.9277786279,0.3647724298,1.6022355639 H,0,1.512140437,-1.2809345636,0.8597238172 H,0,1.6368168056,1.3003575156,-1.1055274492 H,0,1.0410674232,-0.4272734526,-1.4020992224 C,0,-0.3089172808,0.8382971058,-0.3620240055 C,0,3.4292416244,-0.4731520726,0.3393787405 N,0,4.5033711511,-0.5166974719,-0.1263753073 C,0,-1.2856917077,-0.2720248226,-0.2257637399 O,0,-1.0363816986,-1.4486549896,-0.4274204964 O,0,-2.5035103816,0.1685930066,0.1681966281 C,0,-3.5027642416,-0.8518933446,0.3253990113 H,0,-3.6681930609,-1.376168819,-0.6188571336 H,0,-3.1944776306,-1.5787588336,1.0808451379 H,0,-4.4073437956,-0.331818586,0.639332266 C,0,-0.6607790559,2.2063459171,0.1496277434 H,0,0.164950765,2.9055599268,-0.0030656829 H,0,-1.5469176586,2.5974364299,-0.3617508233
MCN + X=H, Y=CN	C,0,-1.2210011207,-0.5675508168,0.7040578946 C,0,0.2016212904,0.925779113,-0.3568746035 H,0,-0.6681563731,-1.4606020437,0.4352504735

	H,0,-1.0947844107,-0.1962526516,1.7145834152 H,0,0.04436927,0.3978300827,-1.2902806932 H,0,-0.4718848756,1.7470613083,-0.142057831 C,0,1.4065193539,0.8530666259,0.2903411676 H,0,1.621201267,1.4926113202,1.1421616827 C,0,-2.4467784476,-0.3283941055,0.0653024786 N,0,-3.4443360702,-0.084883628,-0.4977121398 C,0,2.4050480202,-0.0943846847,-0.0536709476 N,0,3.229593291,-0.8739370587,-0.3243725725
MCN + X=H, Y=CHO	C,0,1.1316663454,-0.3363912151,0.7893954753 C,0,-0.2613126987,0.9245253154,-0.6043600051 H,0,0.9961642992,0.2217396263,1.7083465867 H,0,0.5131674701,-1.2136740308,0.6365660106 H,0,0.4239529941,1.7597229454,-0.6957183906 H,0,-0.1473350866,0.1103402707,-1.3114207247 C,0,-1.4270600121,1.0361263281,0.0997975961 H,0,-1.6511042831,1.9274571541,0.6811275593 C,0,2.3765748263,-0.2614853508,0.1528533555 N,0,3.3996234626,-0.1639294447,-0.4101689746 C,0,-2.3854831236,-0.0737955268,0.1483960738 O,0,-2.1470774888,-1.1927934389,-0.2861641667 H,0,-3.3619017457,0.1503903535,0.6251001412
MCN + X=Me, Y=CN	C,0,-1.5017660703,-0.2129082155,0.8723964799 C,0,-0.0100124284,0.2139330496,-0.8599257743 H,0,-1.0787842318,-1.1705485944,1.1539459935 H,0,-1.2502808534,0.6384295393,1.4945909256 H,0,-0.2792742403,-0.7316125222,-1.3150848751 H,0,-0.5869157008,1.0813787686,-1.1605991897 C,0,1.2249319425,0.3880663674,-0.2879302543 C,0,-2.743100199,-0.2024216039,0.2197228862 N,0,-3.7519670056,-0.1770838094,-0.374679726 C,0,2.0524906308,-0.7524504663,-0.0563735488 N,0,2.7423551529,-1.6700702028,0.1479273035 C,0,1.7448432906,1.720040508,0.1904635582 H,0,1.0397520515,2.518407445,-0.0521137619 H,0,1.9109497057,1.7159865419,1.2741463996 H,0,2.7075132408,1.9524790708,-0.2777386173
MCN + X=H, Y=Ph	C,0,-2.6352909331,-0.1318322738,0.9801391723 C,0,-1.4523496456,-0.8369220945,-0.932751683 H,0,-2.6983585912,-1.1000703146,1.4621323606

	H,0,-1.8620195727,0.5423357655,1.3289169111 H,0,-2.2424908338,-1.5366603986,-1.1786307435 H,0,-1.5659073893,0.1588751932,-1.3461697048 C,0,-0.2455549449,-1.3000340102,-0.4871292504 H,0,-0.1726371771,-2.3552280589,-0.2277045158 C,0,-3.8087121155,0.4201061505,0.4498451277 N,0,-4.7705403127,0.8705890245,-0.0457431163 C,0,0.9618816073,-0.5203707213,-0.2518103291 C,0,2.1169374662,-1.1750595421,0.223541126 C,0,3.2956879227,-0.4752241766,0.4632104482 C,0,3.3501121792,0.9017578542,0.2377329889 C,0,2.2140695232,1.5698945314,-0.2307506617 C,0,1.0365158366,0.8718504974,-0.4731698342 H,0,2.0793265179,-2.2466711359,0.4018357457 H,0,4.1721763064,-1.002921962,0.8275101857 H,0,4.2677579313,1.4510443984,0.4250194526 H,0,2.2492541725,2.640904508,-0.4075841001 H,0,0.1668994481,1.4092715439,-0.8382664059
MCN + X=Me, Y=Ph	C,0,2.6046571463,-0.2059889912,0.9564724467 C,0,1.4045861153,0.6569033206,-0.8884529483 H,0,1.7945139497,-0.8233881602,1.3261565748 H,0,2.2256539033,1.3274122232,-1.1150914934 H,0,1.4546758783,-0.3134500515,-1.3660651647 C,0,0.2317551619,1.1600428767,-0.3860259974 C,0,3.7027623016,-0.8384225716,0.3596407479 N,0,4.6006751352,-1.3542001838,-0.1895824451 C,0,-0.9687780115,0.325887185,-0.1961988339 C,0,-2.204956442,0.9073032162,0.1551115022 C,0,-3.3474112921,0.1302547285,0.3338024858 C,0,-3.2900621249,-1.2544450993,0.1767099181 C,0,-2.0735888362,-1.8535188566,-0.1616866231 C,0,-0.9338001762,-1.0786383251,-0.3441414964 H,0,-2.2799316769,1.9813690129,0.2819971907 H,0,-4.2851920271,0.6102841793,0.5980057977 H,0,-4.1792087066,-1.8610128989,0.3193334367 H,0,-2.0121216642,-2.9314688384,-0.2793967463 H,0,-0.0017758578,-1.5743666126,-0.5931619716 H,0,2.7704012725,0.7408514498,1.4565602167 C,0,0.1789512128,2.6081748714,0.0380166593 H,0,1.1554050081,3.0843925084,-0.0758056967 H,0,-0.5368440855,3.1771849274,-0.5681182149 H,0,-0.1349922696,2.7162794194,1.0831760205

FAc + X=H, Y=Me	C,0,-1.5861827412,-0.4257134624,-0.0186423915 C,0,-0.8287747587,0.8831607618,0.3135834588 C,0,0.435805372,0.743571707,0.9843276602 C,0,1.8248857493,0.5331284912,-0.7499705144 H,0,0.6715494166,-0.1824131687,1.4938320441 H,0,0.8712227141,1.654202908,1.3770845462 H,0,1.2970559262,-0.3311017608,-1.1409051766 H,0,1.5074015767,1.4968188812,-1.1348691797 C,0,3.0757166291,0.3834023089,-0.2112133006 H,0,3.6501014869,1.2772801216,0.0300552836 F,0,-1.0833618944,-0.9792325812,-1.1536903935 F,0,-1.4519814786,-1.349110547,0.9619094334 F,0,-2.8881235203,-0.2048714892,-0.2107377816 O,0,-1.3046461256,1.944967189,-0.0844855159 C,0,3.6883888838,-0.9278780606,0.161582593 H,0,3.8740468689,-0.9885695281,1.2428579467 H,0,3.0525853408,-1.7703526845,-0.1248803489 H,0,4.6653729073,-1.0547011998,-0.3226273467
FAc + X=Me, Y=Me	C,0,2.0069899593,-0.3245056449,-0.0000435941 C,0,1.0897639818,0.8882122203,0.2894599754 C,0,-0.1519165924,0.610473828,0.9546114305 C,0,-1.4850540176,0.1574803659,-0.7933422538 H,0,-0.7107488397,1.4692640273,1.3061902585 H,0,-0.2745304947,-0.3213625094,1.4923215947 H,0,-1.2865187337,1.1405161519,-1.2087953674 H,0,-0.8455487056,-0.6441681647,-1.1461251983 C,0,-2.7156179369,-0.1288627827,-0.2556616454 F,0,1.9595559927,-1.2454306264,0.9914525239 F,0,1.6058490277,-0.9501637227,-1.1383825522 F,0,3.2785884933,0.0475628976,-0.1636550082 O,0,1.4338355481,1.9889916743,-0.1411936839 C,0,-3.7094142113,0.9536749829,0.0545544431 H,0,-3.3633817014,1.9370736826,-0.2729524156 H,0,-4.672484756,0.7489597007,-0.4310951744 H,0,-3.9159199014,1.003119948,1.1328673489 C,0,-3.0953954214,-1.5281540984,0.1364591174 H,0,-4.0276095519,-1.8313381022,-0.3580174635 H,0,-2.3198653133,-2.2531269039,-0.1222121408 H,0,-3.2861525786,-1.5985013881,1.2164085187
FAc + X=Me, Y=OMe	C,0,2.4186034689,-0.2949126252,0.070588965

	F,0,3.6949277219,0.0817438047,-0.0475377046 C,0,1.4775220474,0.9178650807,0.2618481258 O,0,1.8209197798,1.9942937724,-0.2347381796 F,0,2.3345630656,-1.1792578395,1.0943085463 F,0,2.0811640774,-0.9736375284,-1.0599174905 C,0,0.228179156,0.659283263,0.9043071891 C,0,-1.0646450756,0.0767994799,-0.9130212144 C,0,-2.2900521752,-0.2623508371,-0.4051874658 C,0,-2.6579040575,-1.6567270683,0.0068690348 H,0,-0.3879688209,1.5145793776,1.1525752597 H,0,0.0961379604,-0.2463841334,1.4824436884 H,0,-0.9139225661,1.0678450716,-1.3232612778 H,0,-0.3893452526,-0.704237992,-1.2336215544 H,0,-3.5672201916,-2.0051822118,-0.4962795515 H,0,-1.848302803,-2.3424078572,-0.2461217278 H,0,-2.8383689692,-1.7293427138,1.0868384166 O,0,-3.1584387516,0.760776541,-0.1875189458 C,0,-4.45439346,0.5030122623,0.34566506 H,0,-4.935144297,1.477755297,0.4332656697 H,0,-5.0498597036,-0.1292839195,-0.3224852679 H,0,-4.4056067907,0.0386433114,1.3366050198
FAc + X=H, Y=Cl	C,0,2.1582273853,-0.2267170096,0.0406807817 C,0,1.0486356882,0.8444293908,0.1775885799 C,0,-0.1334682842,0.4528581101,0.8990891797 C,0,-1.3889871207,-0.3505761108,-0.7983915397 H,0,-0.8355425144,1.2376105567,1.1539662151 H,0,-0.1113080911,-0.4270917429,1.5300658065 H,0,-1.3800310229,0.6318272718,-1.2568996253 H,0,-0.6282616938,-1.0536558444,-1.1183405451 C,0,-2.5218999408,-0.848142283,-0.2317861862 H,0,-2.6289441658,-1.8726923801,0.1041595733 F,0,2.3265545773,-0.9193761456,1.1896620266 F,0,1.8134783472,-1.1277809099,-0.9182938457 F,0,3.3267612467,0.3145143711,-0.301999442 O,0,1.1988258812,1.9213857179,-0.3945068301 Cl,0,-3.8931007923,0.1456228218,0.1468058631
FAc + X=Me, Y=Cl	C,0,-2.3543244441,0.2660076232,0.0202408801 C,0,-1.3716560944,-0.9087774832,0.2451355777 C,0,-0.1442426424,-0.5993401568,0.9248634739 C,0,1.161459121,-0.0161632411,-0.8308365553 H,0,0.4782305447,-1.4360213545,1.2183972227 H,0,-0.0637064523,0.3153631379,1.4987969705

	H,0,1.0732223361,-1.0216082084,-1.2240007613 H,0,0.4561917366,0.7201850369,-1.199387572 C,0,2.33641704,0.427171763,-0.296512812 F,0,-2.3562618289,1.1309988813,1.0607557918 F,0,-1.9810805134,0.9731759557,-1.0802737284 F,0,-3.602075875,-0.1639715366,-0.1713280575 O,0,-1.6533976449,-2.0026807699,-0.241508376 Cl,0,3.5813115645,-0.7434186699,0.1071741596 C,0,2.6479023167,1.8349272459,0.0944232232 H,0,3.5696088304,2.177479721,-0.3885788103 H,0,1.8309036055,2.499304247,-0.1981840437 H,0,2.8018661367,1.9200767576,1.17679451
FAc + X=Cl, Y=Cl	C,0,-2.5590129551,-0.3023054194,-0.0056130114 C,0,-1.6658202212,0.9239378694,-0.3132179305 C,0,-0.4165855766,0.6604710353,-0.9736825017 C,0,0.929394947,0.2480364566,0.8437680941 H,0,0.1500225099,1.5197170625,-1.3121837564 H,0,-0.2508934176,-0.2879219255,-1.469886648 H,0,0.7413440794,1.2453490033,1.2228252255 H,0,0.2932752282,-0.5553884255,1.1925120858 C,0,2.1571385105,-0.0486999669,0.3391735521 F,0,-2.527810392,-1.209375424,-1.0068388824 F,0,-2.1037719987,-0.9283572829,1.1129379633 F,0,-3.8261630663,0.0515422052,0.2063471922 O,0,-2.0282428588,2.028114236,0.088330049 Cl,0,3.316923924,1.1788923634,-0.0509971898 Cl,0,2.6090299204,-1.6647508891,-0.095737691
FAc + X=H, Y=CO2Me	C,0,2.3436396092,0.5851051156,0.0357924972 C,0,1.9168177236,-0.8292397413,-0.4285938855 C,0,0.6036788711,-0.9519476701,-1.0087585287 C,0,-0.6670908075,-1.2308694815,0.874913317 H,0,0.3624058484,-1.9046102047,-1.4636858684 H,0,0.0712493633,-0.0722301813,-1.3473610313 H,0,-0.0478523241,-2.0535128851,1.2168371035 H,0,-0.3944388261,-0.2375046503,1.2089778768 C,0,-1.9223759292,-1.4749004099,0.3935782177 F,0,1.9271063254,1.5383482668,-0.82705909 F,0,1.7823169109,0.8629819131,1.2405757158 F,0,3.6671376434,0.6795735375,0.1636807672 O,0,2.6808402438,-1.7691633875,-0.2253956113 C,0,-2.901680031,-0.4260786011,0.0515038348 O,0,-4.0500121773,-0.656415319,-0.2770590211

	O,0,-2.3810499207,0.8225994764,0.1377392411 H,0,-2.2708085318,-2.4847633785,0.2025319963 C,0,-3.2991762273,1.8894448164,-0.1550948268 H,0,-3.694198832,1.7892854653,-1.168825704 H,0,-4.133758594,1.8813582782,0.5501924948 H,0,-2.7227504399,2.8085937714,-0.0557640282
FAc + X=Me, Y=CO2Me	C,0,-2.5758023978,-0.5228426806,0.0460530363 C,0,-2.0141123266,0.8403290606,-0.4259450423 C,0,-0.7088803353,0.8278439387,-1.0276525231 C,0,0.6241295791,0.9639617623,0.8571803072 H,0,-0.3711425749,1.7538587387,-1.4765259275 H,0,-0.272109128,-0.1009147308,-1.3713214272 H,0,0.0927816383,1.8442965731,1.2042435891 H,0,0.2551296645,0.0030475651,1.1900288207 C,0,1.892953196,1.0865285936,0.357767041 F,0,-2.250385466,-1.5200357186,-0.8072676883 F,0,-2.049146495,-0.8448287846,1.2557110245 F,0,-3.9035899385,-0.4898859482,0.1691712431 O,0,-2.6747897622,1.8535539839,-0.2041657284 C,0,2.7070844068,-0.1142537979,0.0281824716 O,0,3.8743069325,-0.0641618592,-0.3121108762 O,0,2.0128381263,-1.2721201503,0.1375061478 C,0,2.7644765897,-2.4656657179,-0.1407082753 H,0,3.1554265924,-2.4446376508,-1.160745497 H,0,3.6015461463,-2.5624946617,0.5548830549 H,0,2.0631617292,-3.2897447656,-0.0142710866 C,0,2.5457377929,2.4054460232,0.0684257888 H,0,2.7880392015,2.5003740303,-0.9967105446 H,0,1.9035450847,3.238759813,0.3613998591 H,0,3.4993573403,2.483950263,0.6008347755
FAc + X=H, Y=CN	C,0,1.7826896043,-0.5021581758,0.0331192832 F,0,1.1826705966,-0.9824133485,1.1537475573 F,0,1.6307105676,-1.4336853005,-0.9322837159 F,0,3.0818879518,-0.3573035978,0.2865949789 C,0,1.1289439394,0.8417122683,-0.3714433608 O,0,1.6863378608,1.8894174121,-0.0571906411 C,0,-0.1487243583,0.7660169587,-1.0346957967 C,0,-1.5421302252,0.7749821365,0.8175975447 C,0,-2.8112715969,0.8195726725,0.3067298993 C,0,-3.5516891615,-0.3476076469,-0.0156120006 N,0,-4.1697845685,-1.2979184909,-0.2895692315 H,0,-0.4985002313,-0.1715193017,-1.4494903163

	H,0,-0.5327080725,1.6864002558,-1.4571579341 H,0,-1.1156956735,-0.1585525149,1.1642965009 H,0,-1.0713085099,1.6897299059,1.159314794 H,0,-3.2883296755,1.7695427346,0.0808439086
FAc + X=H, Y=CHO	C,0,2.0313464291,-0.2065305237,0.0588015635 C,0,0.8854885201,0.8314648208,0.1390181345 C,0,-0.2910583402,0.4399242002,0.8687223692 C,0,-1.5269956963,-0.4672420256,-0.8972840696 H,0,-1.0589068779,1.1864524323,1.0328209205 H,0,-0.2640809831,-0.4252887635,1.5190040143 H,0,-1.6414680182,0.5581695125,-1.2326749402 H,0,-0.7015722538,-1.0383093952,-1.3058177924 C,0,-2.5641302627,-1.0842411835,-0.2577869084 H,0,-2.5400171393,-2.1513876019,-0.0492530149 F,0,2.1718280703,-0.8832532377,1.2204964179 F,0,1.7530298418,-1.1226032513,-0.9048570339 F,0,3.1952817234,0.3694487923,-0.2398507311 O,0,1.0091155592,1.891777681,-0.469017871 C,0,-3.7262977542,-0.3187948695,0.2190770063 O,0,-3.7779794035,0.9021155289,0.2146950922 H,0,-4.5744180665,-0.9205951061,0.605116593
FAc + X=Me, Y=CN	C,0,-2.1691525623,-0.3835269719,-0.0644165307 F,0,-3.433303146,-0.06176298,-0.335540932 C,0,-1.3360184163,0.8607663528,0.3275636791 O,0,-1.7306211373,1.9702351342,-0.0238978867 F,0,-1.6329477212,-0.9623510533,-1.1706643746 F,0,-2.1612984462,-1.3131728516,0.9152705554 C,0,-0.0970509844,0.6160325715,1.0173467009 C,0,1.3215490507,0.3697844182,-0.8077168293 C,0,2.5777810724,0.2563314892,-0.2692958547 C,0,3.4592387017,1.4347277982,0.0543732032 C,0,3.076172902,-1.0383109141,0.0725601395 N,0,3.5049121463,-2.0822578603,0.364593266 H,0,0.1044071978,-0.3519511438,1.4593753556 H,0,0.41394548,1.4807709747,1.4226466802 H,0,0.7779769174,-0.5061464212,-1.1390578747 H,0,0.9876703973,1.3298668864,-1.1863903572 H,0,2.9862854041,2.3677820829,-0.2594573957 H,0,3.666438108,1.4889644785,1.1294834913 H,0,4.4266858073,1.3453905915,-0.4516439548

FAc + X=H, Y=Ph	C,0,-3.4213882328,-0.1275715542,-0.0948094625 C,0,-2.1887142044,0.7710609909,-0.3517587236 C,0,-1.0530758027,0.1499314702,-0.9603703257 C,0,0.0386035332,-0.6224976185,0.9962645148 H,0,-0.2247708914,0.7886326134,-1.2401684569 H,0,-1.1445532449,-0.8130868561,-1.4449742396 H,0,0.0071912097,0.3955943852,1.3683486908 H,0,-0.8041340284,-1.2479824922,1.2641155195 C,0,1.1946858148,-1.1884825758,0.5380570975 H,0,1.1805700753,-2.2531789548,0.3093068424 F,0,-3.5646151332,-1.0798118956,-1.0458335701 F,0,-3.2826029477,-0.7722883909,1.0928286864 F,0,-4.5484077141,0.5868744137,-0.0454110517 O,0,-2.2264125078,1.9347109502,0.0543076485 C,0,2.4543161992,-0.5128737166,0.2621952762 C,0,3.5469322704,-1.2715714695,-0.205687619 C,0,4.7720821753,-0.6731877061,-0.483574099 C,0,4.9341052291,0.702245207,-0.304867922 C,0,3.860505406,1.4723237412,0.154976416 C,0,2.6368654784,0.8761872634,0.4363520649 H,0,3.4232665334,-2.342064211,-0.3477523513 H,0,5.6000863563,-1.2778379272,-0.8412747765 H,0,5.8881728937,1.1726485118,-0.5224952163 H,0,3.9809176834,2.5425654711,0.2938510868 H,0,1.8156784313,1.4906705209,0.7916618258
FAc + X=Me, Y=Ph	C,0,-3.3611969384,-0.1698293022,-0.0701306093 C,0,-2.0191937537,-0.6751215784,0.5076548711 C,0,-1.2059643709,0.2918278703,1.174478373 C,0,-0.0416749307,1.0915414742,-0.7266750151 H,0,-0.322375412,-0.0705685309,1.6836116531 H,0,-1.6197380543,1.2446346831,1.4792010363 H,0,-0.2330991264,0.1620313983,-1.246972733 H,0,-0.7664705721,1.8814060094,-0.8882860449 C,0,1.2104424128,1.3933803337,-0.2524213575 F,0,-3.9422988029,0.754956843,0.7293781678 F,0,-3.144386479,0.4255709093,-1.2713388071 F,0,-4.2286390728,-1.1680662213,-0.2537890442 O,0,-1.6886743721,-1.8409952974,0.2711730361 C,0,2.2684026299,0.3735466886,-0.1526829858 C,0,3.6213057808,0.7485096043,-0.019292068 C,0,4.6300005864,-0.2081331737,0.0602880194 C,0,4.3142047284,-1.5670559872,0.0263570272 C,0,2.9777061346,-1.959039594,-0.0851728374

	C,0,1.9673971771,-1.0069052815,-0.1734694585 H,0,3.8914317241,1.7986380381,0.0055010865 H,0,5.6647340057,0.1092111986,0.1504945376 H,0,5.0998620919,-2.3135505058,0.0941416885 H,0,2.718197118,-3.0134092975,-0.0942096445 H,0,0.9364434546,-1.342781262,-0.2231886535 C,0,1.5065861385,2.7966608157,0.2161514819 H,0,2.2409211982,3.2860733165,-0.435758077 H,0,0.6036506357,3.4112569738,0.2085385901 H,0,1.9256635366,2.8065753608,1.2287767763
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