

## "Assessing the Catalytic Potential of Novel Halogen Substituted Carbenes NHCs (F, Cl, Br, I) Catalysts in [3+2] Cycloaddition Reactions: A Computational Investigation"

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Table S1:  $\Delta G_{298}$  (kcal/mol) in the gas phase and solvents for the mononuclear mechanism.

Properties	NHC-F			NHC-Cl		
	Gas	toluene	Water	Gas	toluene	Water
$\Delta G(\text{reagents.})$	0.00	0.00	0.00	0.00	0.00	0.00
$\Delta G(\text{RC}_{\text{Mo}})$	1.31	3.22	4.53	-2.18	-0.65	0.32
$\Delta G(\text{TS1}_{\text{Mo}})$	7.68	11.21	13.94	7.67	10.73	13.05
$\Delta G(\text{IC}_{\text{Mo}})$	-2.02	1.31	3.86	-2.05	0.72	2.79
$\Delta G(\text{TS2}_{\text{Mo}})$	0.50	3.41	5.60	0.68	2.99	4.66
$\Delta G(\text{P}_{\text{Mo}})$	-58.37	-57.68	-57.38	-58.96	-58.06	-57.60
Properties	NHC-Br			NHC-I		
	Gas	toluene	Water	Gas	toluene	Water
$\Delta G(\text{reagents.})$	0.00	0.00	0.00	0.00	0.00	0.00
$\Delta G(\text{RC}_{\text{Mo}})$	-3.58	-1.85	-0.72	-0.08	2.60	4.81
$\Delta G(\text{TS1}_{\text{Mo}})$	7.68	10.86	13.29	14.95	19.06	22.54
$\Delta G(\text{IC}_{\text{Mo}})$	-1.47	1.19	3.16	6.25	9.38	12.00
$\Delta G(\text{TS2}_{\text{Mo}})$	0.04	2.51	4.32	6.93	9.89	12.35
$\Delta G(\text{P}_{\text{Mo}})$	-63.20	-62.12	-61.54	-58.65	-57.04	-55.76

Table S2:  $\Delta G_{298}$  (kcal/mol) in the gas phase and solvents for the binuclear mechanism.

Properties	NHC-F			NHC-Cl		
	Gas	toluene	Water	Gas	toluene	Water
$\Delta G(\text{reagents.})$	0.00	0.00	0.00	0.00	0.00	0.00
$\Delta G(\text{RC}_{\text{Bi}})$	-13.53	-11.12	-9.19	-22.42	-20.73	-19.27

$\Delta G(\text{TS1}_{\text{Bi}})$	3.81	5.95	7.39	-7.82	-6.07	-4.77
$\Delta G(\text{IC}_{\text{Bi}})$	-6.45	-5.66	-5.65	-17.90	-17.45	-17.52
$\Delta G(\text{TS2}_{\text{Bi}})$	0.35	0.50	0.04	-11.98	-11.75	-11.96
$\Delta G(\text{P}_{\text{Bi}})$	-58.81	-58.88	-59.39	-65.77	-66.14	-66.70
Properties	NHC-Br			NHC-I		
	Gas	toluene	Water	Gas	toluene	Water
$\Delta G(\text{reagents.})$	0.00	0.00	0.00	0.00	0.00	0.00
$\Delta G(\text{RC}_{\text{Bi}})$	-10.03	-8.31	-7.02	-0.56	1.38	2.77
$\Delta G(\text{TS1}_{\text{Bi}})$	4.21	6.23	7.65	12.41	14.54	16.01
$\Delta G(\text{IC}_{\text{Bi}})$	-6.19	-5.35	-5.18	3.20	4.32	4.73
$\Delta G(\text{TS2}_{\text{Bi}})$	0.67	0.94	0.74	9.46	9.88	9.77
$\Delta G(\text{P}_{\text{Bi}})$	0.00	-52.61	-52.95	-46.00	-45.42	-45.25

Table S3. ( $E_o$ ) of catalytic cycle components,  $H_{\text{corr}}$ , and  $G_{\text{corr}}$  in the gas phase (in Hartree) for mononuclear CuAAC reaction path.

Compound			
	NHC-F		
	$E_o$	$H_{\text{corr}}$	$G_{\text{corr}}$
$\text{AC}_{\text{Mo}}$	-3044.589387	0.192604	0.114380
$\text{RC}_{\text{Mo}}$	-3479.007209	0.336530	0.240637
$\text{TS1}_{\text{Mo}}$	-3478.999950	0.335521	0.243531
$\text{IC}_{\text{Mo}}$	-3479.018533	0.337473	0.246657
$\text{TS2}_{\text{Mo}}$	-3479.013939	0.336557	0.246077
$\text{P}_{\text{Mo}}$	-3479.110191	0.340329	0.248522
	NHC-Cl		
	$E_o$	$H_{\text{corr}}$	$G_{\text{corr}}$
$\text{AC}_{\text{Mo}}$	-5926.562779	0.179488	0.093028
$\text{RC}_{\text{Mo}}$	-6360.984494	0.324343	0.217619
$\text{TS1}_{\text{Mo}}$	-6360.973931	0.322437	0.222761
$\text{IC}_{\text{Mo}}$	-6360.992349	0.324337	0.225687
$\text{TS2}_{\text{Mo}}$	-6360.987212	0.323860	0.224894
$\text{P}_{\text{Mo}}$	-6361.086923	0.327593	0.229564
	NHC-Br		
	$E_o$	$H_{\text{corr}}$	$G_{\text{corr}}$
$\text{AC}_{\text{Mo}}$	-22828.404587	0.176275	0.079596
$\text{RC}_{\text{Mo}}$	-23262.828139	0.320956	0.203800
$\text{TS1}_{\text{Mo}}$	-23262.815274	0.319070	0.208877
$\text{IC}_{\text{Mo}}$	-23262.832608	0.321440	0.211625
$\text{TS2}_{\text{Mo}}$	-23262.830549	0.320096	0.211974
$\text{P}_{\text{Mo}}$	-23262.935275	0.324254	0.215930
	NHC-I		
	$E_o$	$H_{\text{corr}}$	$G_{\text{corr}}$
$\text{AC}_{\text{Mo}}$	-4607.786163	0.174215	0.069096
$\text{RC}_{\text{Mo}}$	-5042.204208	0.318609	0.193369
$\text{TS1}_{\text{Mo}}$	-5042.185441	0.316632	0.198551
$\text{IC}_{\text{Mo}}$	-5042.202164	0.319021	0.201409
$\text{TS2}_{\text{Mo}}$	-5042.201492	0.318088	0.201824

$P_{Mo}$	-5042.312979	0.321000	0.208802
Azide	-434.3929553	0.143198	0.09931

Table S4. ( $E_o$ ) of catalytic cycle components,  $H_{corr}$ , and  $G_{corr}$  in the gas phase (in Hartree) for binuclear CuAAC reaction path.

Compound	NHC-F		
	$E_o$	$H_{corr}$	$G_{corr}$
$AC_{Bi}$	-5781.735688	0.279004	0.159896
$RC_{Bi}$	-6216.181010	0.423352	0.290015
$TS1_{Bi}$	-6216.158567	0.422149	0.295199
$IC_{Bi}$	-6216.177712	0.423815	0.297994
$TS2_{Bi}$	-6216.167296	0.422624	0.298410
$P_{Bi}$	-6216.257902	0.426359	0.294742
Compound	NHC-Cl		
	$E_o$	$H_{corr}$	$G_{corr}$
$AC_{Bi}$	-11545.694076	0.251959	0.124711
$RC_{Bi}$	-11980.152789	0.397640	0.254050
$TS1_{Bi}$	-11980.133372	0.396319	0.257905
$IC_{Bi}$	-11980.153463	0.398276	0.261924
$TS2_{Bi}$	-11980.144675	0.397360	0.262578
$P_{Bi}$	-11980.228579	0.400411	0.260760
Compound	NHC-Br		
	$E_o$	$H_{corr}$	$G_{corr}$
$AC_{Bi}$	-45349.412270	0.246176	0.099121
$RC_{Bi}$	-45783.848655	0.390886	0.225880
$TS1_{Bi}$	-45783.831590	0.389634	0.231501
$IC_{Bi}$	-45783.851893	0.391558	0.235232
$TS2_{Bi}$	-45783.839927	0.390292	0.234194
$P_{Bi}$	-45783.924498	0.393636	0.233851
Compound	NHC-I		
	$E_o$	$H_{corr}$	$G_{corr}$
$AC_{Bi}$	-8908.180634	0.241757	0.079671
$RC_{Bi}$	-9342.600485	0.386133	0.204979
$TS1_{Bi}$	-9342.585022	0.384675	0.210194
$IC_{Bi}$	-9342.604599	0.386603	0.215085
$TS2_{Bi}$	-9342.592701	0.385348	0.213176
$P_{Bi}$	-9342.684674	0.388806	0.216764

Table S5. ( $E_o$ ) of catalytic cycle components in toluene and water solvents (in Hartree) for mononuclear CuAAC reaction path.

Compound	toluene			
	NHC-F	NHC-Cl	NHC-Br	NHC-I
$AC_{Mo}$	-3044.600192	-5926.571597	-22828.414287	-4607.798530

RC <sub>Mo</sub>	-3479.018193	-6360.994105	-23262.838322	-5042.215538
TS1 <sub>Mo</sub>	-3479.008356	-6360.981120	-23262.823136	-5042.194493
IC <sub>Mo</sub>	-3479.027268	-6360.999997	-23262.841297	-5042.212769
TS2 <sub>Mo</sub>	-3479.023333	-6360.995581	-23262.839550	-5042.212379
P <sub>Mo</sub>	-3479.123137	-6361.097537	-23262.946496	-5042.326022

Azide -434.3961909

Compound	water			
	NHC-F	NHC-Cl	NHC-Br	NHC-I
AC <sub>Mo</sub>	-3044.609501	-5926.579164	-22828.422461	-4607.809266
RC <sub>Mo</sub>	-3479.027949	-6361.002656	-23262.847232	-5042.225292
TS1 <sub>Mo</sub>	-3479.015848	-6360.987513	-23262.829983	-5042.202218
IC <sub>Mo</sub>	-3479.035043	-6361.006792	-23262.848875	-5042.221872
TS2 <sub>Mo</sub>	-3479.031685	-6361.003010	-23262.847374	-5042.221729
P <sub>Mo</sub>	-3479.134496	-6361.106906	-23262.956285	-5042.337241

Azide -434.3987224

Table S6. ( $E_0$ ) of catalytic cycle components in toluene and water solvents (in Hartree) for binuclear CuAAC reaction path.

Compound	toluene			
	NHC-F	NHC-Cl	NHC-Br	NHC-I
AC <sub>Bi</sub>	-5781.771961	-11545.724278	-45349.442470	-8908.212494
RC <sub>Bi</sub>	-6216.216682	-11980.183533	-45783.879351	-9342.632476
TS1 <sub>Bi</sub>	-6216.194657	-11980.164027	-45783.861796	-9342.616719
IC <sub>Bi</sub>	-6216.215960	-11980.186186	-45783.883986	-9342.637906
TS2 <sub>Bi</sub>	-6216.206554	-11980.177757	-45783.872918	-9342.627137
P <sub>Bi</sub>	-6216.297523	-11980.262612	-45783.957917	-9342.718842

Compound	water			
	NHC-F	NHC-Cl	NHC-Br	NHC-I
AC <sub>Bi</sub>	-5781.798892	-11545.746591	-45349.464378	-8908.235490
RC <sub>Bi</sub>	-6216.243075	-11980.206058	-45783.901730	-9342.655792
TS1 <sub>Bi</sub>	-6216.221835	-11980.186798	-45783.883987	-9342.639910
IC <sub>Bi</sub>	-6216.245406	-11980.211141	-45783.908163	-9342.662783
TS2 <sub>Bi</sub>	-6216.236748	-11980.202933	-45783.897691	-9342.652831
P <sub>Bi</sub>	-6216.327791	-11980.288342	-45783.982898	-9342.744107

Table S7:  $\Delta G_{298}$  in the gas phase and in toluene or water as a solvent for uncatalyzed pathway (in kcal/mol).

Compound	1-4			1-5		
	Gas	Toluene	Water	Gas	Toluene	Water
$\Delta G$ (reagents)	0.0	0.0	0.0	0.0	0.0	0.0
$\Delta G$ (TS)	32.3	32.9	33.3	30.6	31.5	32.3
$\Delta G$ (P)	-62.1	-62.7	-63.5	-59.8	-60.2	-60.6

Table S8. ( $E_o$ ) in the in toluene and water as a solvent for uncatalyzed cycle components,  $H_{\text{corr}}$ , and  $G_{\text{corr}}$  in the gas phase (in Hartree).

Compound	MN12L				
	$E_o$ gas phase	$E_o$ toluene	$E_o$ water	$H_{\text{corr}}$	$G_{\text{corr}}$
Azide	-434.392955	-434.396191	-434.398722	0.143198	0.099310
alkyne	-307.868657	-307.871284	-307.873359	0.117950	0.080250
1,4-TS	-742.231141	-742.236017	-742.240038	0.261346	0.200499
1,5-TS	-742.234612	-742.238895	-742.242335	0.261262	0.201247
1,4-P	-742.389283	-742.396116	-742.401878	0.267302	0.208233
1,5-P	-742.387732	-742.394211	-742.399565	0.267447	0.210414

Table S9. ( $E_o$ ) of catalytic cycle components in solvents (in Hartree) for mononuclear CuAAC reaction path.

	$E_o$		
	NHC-F		
	$AC_{\text{MO}}$	$RC_{\text{MO}}$	$TS1_{\text{MO}}$
methanol	-3044.609057	-3479.015483	-3479.015483
acetonitrile	-3044.609123	-3479.027544	-3479.015537
cyclohexane	-3044.598655	-3479.016617	-3479.007147
benzene	-3044.599793	-3479.017783	-3479.008041
dichloromethane	-3044.607087	-3479.025378	-3479.013872
	NHC-Cl		
	$AC_{\text{MO}}$	$RC_{\text{MO}}$	$TS1_{\text{MO}}$
methanol	-5926.578803	-6360.987200	-6360.987200
acetonitrile	-5926.578856	-6361.002299	-6360.987246
cyclohexane	-5926.570349	-6360.992727	-6360.980089
benzene	-5926.571273	-6360.993746	-6360.980851
dichloromethane	-5926.577198	-6361.000394	-6360.985823
	NHC-Br		
	$AC_{\text{MO}}$	$RC_{\text{MO}}$	$TS1_{\text{MO}}$
methanol	-22828.422072	-23262.829651	-23262.829651
acetonitrile	-22828.422129	-23262.846861	-23262.829700
cyclohexane	-22828.412928	-23262.836875	-23262.822022
benzene	-22828.413934	-23262.837945	-23262.822847
dichloromethane	-22828.420344	-23262.844884	-23262.828183
	NHC-I		
	$AC_{\text{MO}}$	$RC_{\text{MO}}$	$TS1_{\text{MO}}$
methanol	-4607.808745	-5042.201845	-5042.201845
acetonitrile	-4607.808822	-5042.224888	-5042.201900
cyclohexane	-4607.796778	-5042.213942	-5042.193223
benzene	-4607.798074	-5042.215123	-5042.194163
dichloromethane	-4607.806447	-5042.222732	-5042.200197

Table S10. ( $E_o$ ) of catalytic cycle components in solvents (in Hartree) for binuclear CuAAC reaction path.

	$E_o$		
	NHC-F		

	<b>AC<sub>MO</sub></b>	<b>RC<sub>MO</sub></b>	<b>TS1<sub>MO</sub></b>
methanol	-5781.797681	-6216.220603	-6216.220603
acetonitrile	-5781.797860	-6216.242066	-6216.220785
cyclohexane	-5781.767172	-6216.211977	-6216.189864
benzene	-5781.770727	-6216.215469	-6216.193421
dichloromethane	-5781.792219	-6216.236548	-6216.215061
<b>NHC-CI</b>			
	<b>AC<sub>BI</sub></b>	<b>RC<sub>BI</sub></b>	<b>TS1<sub>BI</sub></b>
methanol	-11545.745589	-11980.185773	-11980.185773
acetonitrile	-11545.745736	-11980.205201	-11980.185924
cyclohexane	-11545.720303	-11980.179497	-11980.159981
benzene	-11545.723254	-11980.182494	-11980.162984
dichloromethane	-11545.741066	-11980.200508	-11980.181151
<b>NHC-Br</b>			
	<b>AC<sub>BI</sub></b>	<b>RC<sub>BI</sub></b>	<b>TS1<sub>BI</sub></b>
methanol	-45349.463404	-45783.882993	-45783.882993
acetonitrile	-45349.463548	-45783.900880	-45783.883140
cyclohexane	-45349.438524	-45783.875331	-45783.857828
benzene	-45349.441454	-45783.878316	-45783.860774
dichloromethane	-45349.458998	-45783.896226	-45783.878508
<b>NHC-I</b>			
	<b>AC<sub>BI</sub></b>	<b>RC<sub>BI</sub></b>	<b>TS1<sub>BI</sub></b>
methanol	-8908.234471	-9342.638874	-9342.638874
acetonitrile	-8908.234621	-9342.654907	-9342.639027
cyclohexane	-8908.208339	-9342.628286	-9342.612562
benzene	-8908.211425	-9342.631397	-9342.615649
dichloromethane	-8908.229856	-9342.650058	-9342.634195

Table S11. ( $E_o$ ) of Azide in solvents (in Hartree) for mononuclear CuAAC reaction path.

<b>E<sub>o</sub></b>	
<b>Azide</b>	
methanol	-434.398606
acetonitrile	-434.398623
cyclohexane	-434.395752
benzene	-434.396077
dichloromethane	-434.398085

### MN12L Optimized Cartesian Coordinates for mononuclear catalytic cycle components

Azide

7	-2.679814000	-1.130672000	1.175397000
7	-2.272638000	0.338471000	-0.613110000
7	-2.427365000	-0.396209000	0.354994000
6	0.191276000	0.566889000	-0.293159000
6	1.177301000	1.229108000	0.440646000
6	0.455186000	-0.717625000	-0.777489000
6	2.409428000	0.627434000	0.676936000

1	0.972529000	2.229930000	0.835808000
6	1.684245000	-1.322020000	-0.535867000
1	-0.314370000	-1.245148000	-1.350771000
6	2.665367000	-0.650902000	0.189489000
1	3.171351000	1.156949000	1.255347000
1	1.878183000	-2.327967000	-0.917956000
1	3.629829000	-1.128681000	0.380834000
6	-1.127626000	1.242734000	-0.571945000
1	-1.114778000	1.728347000	-1.560052000
1	-1.295078000	2.051739000	0.164155000

AC<sub>Mo</sub>\_NHC-F

6	-2.172778000	-0.000064000	-0.000053000
6	-3.404803000	-0.000112000	-0.000078000
29	-0.335679000	0.000029000	0.000004000
6	-4.823184000	-0.000032000	-0.000045000
6	-5.547411000	-1.208514000	-0.000214000
6	-5.547301000	1.208509000	0.000168000
6	-6.935363000	-1.203918000	-0.000222000
6	-6.935255000	1.204032000	0.000234000
6	-7.637254000	0.000090000	0.000020000
1	-4.993666000	-2.150989000	-0.000394000
1	-4.993481000	2.150940000	0.000320000
1	-7.479005000	-2.153050000	-0.000415000
1	-7.478814000	2.153212000	0.000451000
1	-8.730534000	0.000141000	0.000046000
9	2.549437000	3.035136000	1.064455000
6	2.038923000	2.458269000	-0.000002000
9	2.549379000	3.035119000	-1.064490000
9	0.746653000	2.589831000	0.000026000
7	2.398310000	1.063483000	-0.000012000
6	1.535673000	0.000012000	-0.000020000
7	2.398270000	-1.063495000	-0.000024000
6	2.038833000	-2.458266000	0.000091000
9	0.746558000	-2.589778000	0.000146000
9	2.549261000	-3.035217000	-1.064363000
9	2.549335000	-3.035063000	1.064585000
9	4.679843000	-1.544023000	-0.000084000
6	3.726685000	-0.670503000	-0.000078000
6	3.726710000	0.670438000	-0.000067000
9	4.679899000	1.543923000	-0.000085000

TS1<sub>Mo</sub>\_NHC-F

7	-0.884160000	0.799083000	1.415069000
7	-2.054871000	0.937765000	1.919610000
7	-3.171025000	0.741170000	1.607468000
6	-2.410138000	-0.145420000	-0.669680000
6	-3.571584000	0.002754000	-0.190472000

29	-0.608505000	0.071412000	-0.416135000
6	0.223605000	1.240958000	2.241569000
1	0.637922000	2.195939000	1.860306000
1	-0.132898000	1.454350000	3.264971000
6	1.321910000	0.209491000	2.276873000
6	2.663402000	0.592013000	2.206096000
6	1.012040000	-1.152056000	2.363206000
6	3.678820000	-0.363457000	2.218491000
6	2.023374000	-2.105215000	2.373238000
6	3.360705000	-1.716602000	2.291761000
1	2.913565000	1.657191000	2.130981000
1	-0.038700000	-1.459174000	2.395014000
1	4.724919000	-0.047442000	2.159047000
1	1.767124000	-3.167358000	2.429162000
1	4.153208000	-2.470007000	2.288674000
6	-5.002309000	-0.120833000	-0.244041000
6	-5.868424000	0.686459000	0.509276000
6	-5.558902000	-1.082053000	-1.108379000
6	-7.245168000	0.533029000	0.397091000
6	-6.934638000	-1.227694000	-1.213524000
6	-7.785885000	-0.421549000	-0.460085000
1	-5.448975000	1.437758000	1.180034000
1	-4.884516000	-1.713673000	-1.693131000
1	-7.906905000	1.172245000	0.988404000
1	-7.348222000	-1.981198000	-1.889680000
1	-8.869942000	-0.537380000	-0.542211000
9	1.562095000	-2.619639000	-2.273363000
6	1.692062000	-2.321529000	-0.997259000
9	2.591227000	-3.125000000	-0.479864000
9	0.545190000	-2.497433000	-0.401383000
7	2.120983000	-0.957254000	-0.849226000
6	1.239227000	0.093778000	-0.808930000
7	2.067178000	1.173750000	-0.960130000
6	1.675312000	2.549154000	-0.919608000
9	0.387747000	2.648116000	-0.754345000
9	2.293127000	3.154482000	0.078353000
9	2.031976000	3.148015000	-2.033407000
9	4.328000000	1.696714000	-1.202986000
6	3.395800000	0.802909000	-1.094446000
6	3.431783000	-0.534366000	-1.032021000
9	4.425903000	-1.359971000	-1.073911000

TS1'<sub>Mo</sub>\_NHC-F

7	0.303158000	-0.962249000	-1.035056000
7	-0.803973000	-1.232380000	-1.355492000
7	-1.960467000	-1.272840000	-0.872165000
6	-0.907623000	-0.097839000	1.280910000
6	-2.071856000	-0.479202000	0.943331000
29	0.821345000	-0.093092000	0.719436000



6	-3.476676000	-0.592682000	1.252073000
6	-4.158580000	-1.813057000	1.131762000
6	-4.194144000	0.544550000	1.658014000
6	-5.522100000	-1.888617000	1.389964000
6	-5.555997000	0.462419000	1.915312000
6	-6.228172000	-0.750621000	1.775350000
1	-3.594916000	-2.700916000	0.827317000
1	-3.661967000	1.496670000	1.742890000
1	-6.039800000	-2.847599000	1.294647000
1	-6.103288000	1.359426000	2.219131000
1	-7.301769000	-0.810942000	1.973540000
9	3.914859000	2.977661000	1.478622000
6	3.105349000	2.508674000	0.554692000
9	3.232912000	3.258041000	-0.518239000
9	1.877852000	2.549353000	0.980194000
7	3.476038000	1.157271000	0.235560000
6	2.691698000	0.049590000	0.389141000
7	3.518143000	-0.952565000	-0.035732000
6	3.162690000	-2.348494000	-0.106321000
9	2.104090000	-2.576390000	0.613540000
9	2.953144000	-2.704916000	-1.348497000
9	4.169890000	-3.056628000	0.362959000
9	5.663985000	-1.264816000	-0.923468000
6	4.751519000	-0.476241000	-0.456733000
6	4.726055000	0.852473000	-0.279184000
9	5.604580000	1.778896000	-0.492523000
6	-3.108002000	-1.222618000	-1.771399000
1	-2.755455000	-1.395404000	-2.801568000
6	-3.846271000	0.088305000	-1.670086000
6	-3.145936000	1.292171000	-1.555136000
6	-5.240511000	0.105486000	-1.648310000
6	-3.834836000	2.492055000	-1.419173000
6	-5.930600000	1.306822000	-1.518734000
6	-5.228571000	2.502657000	-1.399136000
1	-2.050216000	1.280373000	-1.530562000
1	-5.789814000	-0.841697000	-1.699912000
1	-3.279123000	3.428516000	-1.318222000
1	-7.023806000	1.306199000	-1.489609000
1	-5.767923000	3.446767000	-1.283206000
1	-3.797643000	-2.048166000	-1.529231000

AC<sub>Bi</sub>\_NHC-F

6	0.001884000	2.054818000	0.000754000
6	0.003909000	3.297298000	0.000969000
29	-1.255529000	0.639704000	0.000337000
6	0.006140000	4.710076000	0.000867000
6	0.007279000	5.421777000	1.217295000
6	0.007296000	5.421601000	-1.215665000
6	0.009548000	6.807813000	1.210524000

6	0.009565000	6.807638000	-1.209099000
6	0.010695000	7.501142000	0.000662000
1	0.006367000	4.866632000	2.158679000
1	0.006397000	4.866318000	-2.156968000
1	0.010431000	7.356401000	2.155644000
1	0.010462000	7.356087000	-2.154299000
1	0.012486000	8.594421000	0.000582000
6	-2.968535000	-1.003859000	-2.459357000
7	-3.243388000	-1.258316000	-1.061792000
6	-2.617764000	-0.680192000	-0.000195000
7	-3.243763000	-1.258797000	1.060920000
6	-2.969303000	-1.005070000	2.458696000
6	-4.218229000	-2.162437000	0.671299000
6	-4.217999000	-2.162123000	-0.672926000
29	1.255960000	0.636687000	0.000351000
6	2.615457000	-0.686016000	0.000095000
7	3.240005000	-1.265953000	1.061339000
6	2.965690000	-1.011825000	2.459062000
6	4.213133000	-2.171124000	0.671921000
6	4.213417000	-2.170560000	-0.672302000
7	3.240463000	-1.265052000	-1.061370000
6	2.966639000	-1.009841000	-2.458995000
9	2.578683000	-2.121747000	-3.030185000
9	2.027536000	-0.108369000	-2.558697000
9	4.057529000	-0.588365000	-3.040866000
9	2.026335000	-0.110656000	2.559142000
9	4.056296000	-0.590510000	3.041587000
9	2.577830000	-2.124247000	3.029305000
9	4.903320000	-2.817074000	1.546471000
9	4.903958000	-2.815795000	-1.547099000
9	-2.029088000	-0.104814000	2.558912000
9	-2.582533000	-2.117904000	3.028883000
9	-4.059543000	-0.582761000	3.041177000
9	-4.909756000	-2.807168000	1.545689000
9	-4.909249000	-2.806412000	-1.547859000
9	-2.581900000	-2.116463000	-3.030085000
9	-4.058534000	-0.580953000	-3.041858000
9	-2.028081000	-0.103770000	-2.558840000

TS1<sub>Bi</sub>\_NHC-F

29	-0.583795000	1.327010000	-0.173961000
6	1.910587000	2.915635000	-0.231475000
6	1.201477000	1.860901000	-0.237645000
7	0.665928000	4.373951000	-0.002899000
7	-1.267482000	3.137030000	0.058140000
7	-0.472696000	4.125692000	0.068111000
6	-3.338721000	2.435353000	1.139168000
6	-2.713424000	2.120820000	2.349633000
6	-4.559529000	1.829135000	0.830324000

6	-3.292175000	1.208254000	3.225016000
1	-1.754822000	2.588798000	2.598930000
6	-5.139105000	0.913046000	1.706416000
1	-5.065871000	2.084277000	-0.107349000
6	-4.501137000	0.592400000	2.902540000
1	-2.794323000	0.971819000	4.170053000
1	-6.099857000	0.453286000	1.455947000
1	-4.954297000	-0.124046000	3.593234000
6	-2.699013000	3.400736000	0.175490000
1	-2.852404000	4.443039000	0.502338000
1	-3.182119000	3.310445000	-0.816283000
6	3.200003000	3.541273000	-0.352938000
6	4.227903000	2.778129000	-0.941250000
6	3.489746000	4.836113000	0.099803000
6	5.506005000	3.297855000	-1.069638000
1	3.992980000	1.773772000	-1.308897000
6	4.775570000	5.346015000	-0.030582000
1	2.705173000	5.438241000	0.559033000
6	5.784855000	4.585536000	-0.613866000
1	6.291999000	2.697874000	-1.535496000
1	4.991533000	6.355217000	0.329105000
1	6.792072000	4.997200000	-0.716996000
6	-2.019513000	0.060729000	-0.240164000
7	-2.344296000	-0.894578000	0.676017000
7	-2.941968000	-0.127225000	-1.217819000
6	-3.432121000	-1.657994000	0.266042000
6	-3.815697000	-1.161658000	-0.921089000
9	-3.907024000	-2.612163000	0.990481000
9	-4.787356000	-1.457043000	-1.716291000
6	-1.485271000	-1.263485000	1.768627000
9	-2.194977000	-1.689581000	2.774551000
9	-0.678198000	-2.243664000	1.382789000
9	-0.747492000	-0.248601000	2.128954000
6	-3.077181000	0.671908000	-2.409359000
9	-4.219059000	1.318492000	-2.381647000
9	-2.092945000	1.528388000	-2.471882000
9	-3.061263000	-0.109306000	-3.457750000
29	1.429354000	-0.035330000	-0.240073000
6	2.017996000	-1.849293000	-0.170718000
7	1.450957000	-3.006346000	-0.613293000
7	3.181701000	-2.285898000	0.382861000
6	4.186544000	-1.457674000	1.020169000
9	3.836004000	-0.202841000	0.919537000
9	5.334331000	-1.650638000	0.427062000
9	4.288615000	-1.794403000	2.278135000
6	3.332601000	-3.658708000	0.288617000
9	4.372813000	-4.246175000	0.767767000
6	2.239002000	-4.115306000	-0.344952000
9	1.865649000	-5.294613000	-0.703783000
6	0.207774000	-3.139034000	-1.333304000

9	0.445156000	-3.575730000	-2.541759000
9	-0.565083000	-3.996345000	-0.715610000
9	-0.393540000	-1.975900000	-1.394291000

TS1'Bi\_NHC-F

29	-0.113664000	-1.460019000	0.779298000
6	-2.661033000	0.054652000	0.698148000
6	-1.414097000	-0.140296000	0.518678000
7	-3.456835000	-1.569448000	1.492923000
7	-1.456517000	-2.691236000	1.548927000
7	-2.598435000	-2.454016000	1.620061000
6	-3.812726000	0.915640000	0.571764000
6	-4.628911000	1.212868000	1.672208000
6	-4.121001000	1.461189000	-0.684442000
6	-5.738918000	2.033310000	1.514125000
1	-4.376658000	0.793041000	2.651317000
6	-5.233185000	2.278161000	-0.833473000
1	-3.491646000	1.206184000	-1.542709000
6	-6.047078000	2.561789000	0.261859000
1	-6.368146000	2.267318000	2.377038000
1	-5.475278000	2.689171000	-1.817248000
1	-6.924930000	3.201752000	0.140287000
6	1.676398000	-2.169428000	0.663086000
7	2.798542000	-1.662808000	1.248908000
7	2.180320000	-3.059369000	-0.227330000
6	3.960276000	-2.184930000	0.695152000
6	3.564988000	-3.076390000	-0.230114000
9	5.129962000	-1.806368000	1.080392000
9	4.217984000	-3.863243000	-1.014672000
6	2.776764000	-0.579451000	2.195838000
9	3.734510000	-0.737649000	3.065319000
9	2.964876000	0.567822000	1.563004000
9	1.620492000	-0.540883000	2.796619000
6	1.404376000	-3.890150000	-1.122741000
9	1.682189000	-5.146195000	-0.896034000
9	0.135233000	-3.665543000	-0.925703000
9	1.724154000	-3.599098000	-2.359599000
29	0.060157000	0.927257000	-0.012544000
6	1.431562000	2.162473000	-0.480996000
7	2.666523000	1.975631000	-1.031456000
7	1.408136000	3.507372000	-0.274102000
6	0.316082000	4.265307000	0.304947000
9	-0.687667000	3.466100000	0.540932000
9	-0.042180000	5.200917000	-0.534112000
9	0.720553000	4.818561000	1.418183000
6	2.580647000	4.129166000	-0.670491000
9	2.734665000	5.400342000	-0.537787000
6	3.377454000	3.160562000	-1.150801000
9	4.566005000	3.167886000	-1.648813000

6	3.231713000	0.729363000	-1.473767000
9	3.532188000	0.807585000	-2.742213000
9	4.327820000	0.467600000	-0.797044000
9	2.371228000	-0.239776000	-1.279746000
6	-4.868491000	-1.911538000	1.295819000
1	-4.998826000	-2.974962000	1.553935000
1	-5.472292000	-1.332343000	2.011391000
6	-5.316740000	-1.620941000	-0.112143000
6	-4.498221000	-1.937643000	-1.199470000
6	-6.546337000	-1.002921000	-0.335975000
6	-4.905316000	-1.631992000	-2.493274000
6	-6.957412000	-0.704857000	-1.631506000
6	-6.134636000	-1.012409000	-2.711395000
1	-3.522786000	-2.409448000	-1.030761000
1	-7.178681000	-0.733538000	0.517618000
1	-4.260711000	-1.881573000	-3.340392000
1	-7.921869000	-0.217427000	-1.797471000
1	-6.453680000	-0.772682000	-3.729134000

#### AC<sub>Mo</sub>\_NHC-Cl

6	-2.853851000	0.000038000	-0.000056000
6	-4.086416000	-0.000002000	0.000111000
29	-1.002741000	0.000172000	-0.000111000
6	-5.505420000	-0.000068000	0.000087000
6	-6.230289000	-0.613769000	-1.040468000
6	-6.230483000	0.613506000	1.040575000
6	-7.618418000	-0.610174000	-1.037304000
6	-7.618607000	0.609684000	1.037277000
6	-8.321334000	-0.000303000	-0.000047000
1	-5.677321000	-1.092572000	-1.852854000
1	-5.677672000	1.092399000	1.853015000
1	-8.161285000	-1.091375000	-1.856038000
1	-8.161637000	1.090793000	1.855956000
1	-9.414568000	-0.000390000	-0.000088000
17	2.010660000	3.292422000	1.387661000
6	1.345008000	2.477319000	-0.057353000
17	2.011532000	3.223500000	-1.538404000
17	-0.396108000	2.690994000	-0.063073000
7	1.734221000	1.078503000	-0.024121000
6	0.884743000	0.000029000	-0.000136000
7	1.734213000	-1.078479000	0.024028000
6	1.344883000	-2.477223000	0.056832000
17	-0.396164000	-2.690672000	0.063250000
17	2.011147000	-3.292304000	-1.387558000
17	2.011999000	-3.224041000	1.538427000
17	4.443711000	-1.661245000	0.037179000
6	3.070625000	-0.674921000	0.015139000
6	3.070604000	0.674943000	-0.015121000
17	4.443615000	1.661443000	-0.037090000

TS1<sub>Mo</sub>\_NHC-Cl

7	-1.448768000	0.604009000	1.674755000
7	-2.640813000	0.703067000	2.130971000
7	-3.740285000	0.542069000	1.744240000
6	-2.859305000	-0.046944000	-0.591152000
6	-4.041012000	0.038449000	-0.145899000
29	-1.057088000	0.079906000	-0.202397000
6	-0.380811000	1.048961000	2.548831000
1	0.040004000	2.004050000	2.172018000
1	-0.781862000	1.265419000	3.554931000
6	0.723712000	0.028084000	2.626171000
6	2.063560000	0.420748000	2.613670000
6	0.419459000	-1.335388000	2.689848000
6	3.084444000	-0.526955000	2.655802000
6	1.435697000	-2.280557000	2.738721000
6	2.772505000	-1.881281000	2.711946000
1	2.309817000	1.486716000	2.548814000
1	-0.629758000	-1.648685000	2.678676000
1	4.129793000	-0.203164000	2.620788000
1	1.185625000	-3.344852000	2.778628000
1	3.570117000	-2.629923000	2.726787000
6	-5.467895000	-0.071775000	-0.286273000
6	-6.372114000	0.644751000	0.512692000
6	-5.979872000	-0.922059000	-1.284039000
6	-7.741422000	0.511465000	0.315581000
6	-7.348586000	-1.048791000	-1.473325000
6	-8.237693000	-0.333643000	-0.673147000
1	-5.988240000	1.310080000	1.287338000
1	-5.276634000	-1.483254000	-1.905566000
1	-8.432502000	1.079337000	0.944956000
1	-7.726795000	-1.716117000	-2.252879000
1	-9.316145000	-0.435089000	-0.821406000
17	1.423062000	-2.416508000	-2.674427000
6	1.242804000	-2.314504000	-0.888518000
17	2.199102000	-3.629361000	-0.162837000
17	-0.436761000	-2.598164000	-0.438346000
7	1.688088000	-0.993670000	-0.482018000
6	0.825405000	0.089566000	-0.471218000
7	1.662900000	1.181021000	-0.505382000
6	1.259760000	2.557229000	-0.667160000
17	-0.483795000	2.754880000	-0.653486000
17	1.941018000	3.562944000	0.657154000
17	1.894535000	3.163099000	-2.229702000
17	4.365126000	1.784334000	-0.519717000
6	3.001194000	0.783304000	-0.567865000
6	3.014445000	-0.563977000	-0.578289000
17	4.417633000	-1.505775000	-0.632744000

TS1<sub>Mo</sub>\_NHC-Cl

7	-0.650604000	-0.041930000	-1.458536000
7	-1.805124000	-0.126291000	-1.693854000
7	-2.900888000	-0.198016000	-1.079883000
6	-1.417955000	-0.462351000	1.106101000
6	-2.663065000	-0.501585000	0.861246000
29	0.234425000	-0.224136000	0.346780000
6	-4.027557000	-0.618968000	1.327014000
6	-4.795845000	0.529655000	1.577737000
6	-4.618768000	-1.877046000	1.516572000
6	-6.110400000	0.421292000	2.010490000
6	-5.936539000	-1.980763000	1.951201000
6	-6.686388000	-0.834115000	2.198962000
1	-4.342103000	1.511612000	1.414677000
1	-4.021912000	-2.774719000	1.328384000
1	-6.695906000	1.326630000	2.196023000
1	-6.380693000	-2.968971000	2.102177000
1	-7.722556000	-0.917747000	2.538297000
17	3.070422000	3.236523000	1.763344000
6	2.330274000	2.493635000	0.313098000
17	2.745244000	3.460807000	-1.134709000
17	0.587158000	2.506984000	0.510151000
7	2.857672000	1.155195000	0.150262000
6	2.126492000	-0.007233000	0.152714000
7	3.074195000	-0.981809000	-0.046169000
6	2.825009000	-2.403768000	-0.139174000
17	1.119437000	-2.792994000	0.008391000
17	3.404389000	-2.994917000	-1.726276000
17	3.712013000	-3.237712000	1.171725000
17	5.812120000	-1.265329000	-0.376996000
6	4.355554000	-0.434886000	-0.152202000
6	4.220001000	0.901826000	-0.030350000
17	5.477842000	2.031631000	-0.083718000
6	-4.050044000	-0.801731000	-1.730705000
1	-3.829713000	-0.922924000	-2.804646000
1	-4.203502000	-1.821313000	-1.325899000
6	-5.306913000	0.001891000	-1.534615000
6	-5.275471000	1.397758000	-1.579925000
6	-6.520296000	-0.643074000	-1.298481000
6	-6.438890000	2.133174000	-1.384831000
6	-7.686999000	0.091499000	-1.109624000
6	-7.648529000	1.482118000	-1.147801000
1	-4.318974000	1.904018000	-1.745259000
1	-6.542849000	-1.736980000	-1.232750000
1	-6.403283000	3.225983000	-1.415308000
1	-8.630060000	-0.426223000	-0.912745000
1	-8.562170000	2.061693000	-0.989384000

AC<sub>Bi</sub>\_NHC-Cl

6	0.000767000	2.475105000	-0.000541000
6	0.001995000	3.717135000	-0.000567000
29	1.257912000	1.041001000	-0.001227000
6	0.003535000	5.132108000	-0.000865000
6	0.001791000	5.845820000	-1.215647000
6	0.006882000	5.846333000	1.213604000
6	0.003357000	7.232213000	-1.210100000
6	0.008469000	7.232734000	1.207456000
6	0.006710000	7.927124000	-0.001468000
1	-0.000798000	5.291470000	-2.157506000
1	0.008208000	5.292410000	2.155716000
1	0.001977000	7.779698000	-2.155954000
1	0.011084000	7.780615000	2.153079000
1	0.007965000	9.020339000	-0.001699000
6	2.985914000	-0.565028000	2.472988000
7	3.228393000	-0.879247000	1.072145000
6	2.629598000	-0.289843000	-0.003073000
7	3.222264000	-0.883311000	-1.079464000
6	2.972735000	-0.573623000	-2.480055000
6	4.156273000	-1.842132000	-0.680904000
6	4.159865000	-1.839840000	0.671912000
29	-1.257723000	1.042213000	0.000706000
6	-2.630555000	-0.287452000	0.003176000
7	-3.229766000	-0.876889000	-1.071809000
6	-2.986883000	-0.563667000	-2.472780000
6	-4.161765000	-1.836794000	-0.671195000
6	-4.158171000	-1.838533000	0.681623000
7	-3.223665000	-0.880023000	1.079785000
6	-2.973914000	-0.569842000	2.480252000
17	-2.351536000	-2.025198000	3.290093000
17	-1.784236000	0.727677000	2.665652000
17	-4.491227000	-0.033809000	3.231223000
17	-1.801595000	0.737628000	-2.661091000
17	-4.508360000	-0.029974000	-3.216713000
17	-2.364376000	-2.016354000	-3.287342000
17	-5.103482000	-2.822222000	-1.662795000
17	-5.096154000	-2.825112000	1.675625000
17	1.783674000	0.724315000	-2.666164000
17	2.349799000	-2.029114000	-3.289259000
17	4.490351000	-0.038589000	-3.231137000
17	5.093721000	-2.829629000	-1.674488000
17	5.101300000	-2.825086000	1.663927000
17	2.363260000	-2.016999000	3.288659000
17	4.507707000	-0.031362000	3.216271000
17	1.800914000	0.736630000	2.660713000

RC<sub>Bi</sub>\_NHC-Cl

29	-0.673254000	1.854369000	-0.085490000
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6	2.139791000	3.110281000	-0.666264000
6	0.966981000	2.737969000	-0.458467000
7	-0.905787000	5.344067000	1.228216000
7	-1.883475000	3.238423000	0.824837000
7	-1.441677000	4.372493000	1.045215000
6	-3.786411000	2.066842000	1.892261000
6	-3.449612000	2.259249000	3.235605000
6	-4.652708000	1.024495000	1.550262000
6	-4.021327000	1.463684000	4.222463000
1	-2.763990000	3.067465000	3.513478000
6	-5.210274000	0.214256000	2.536981000
1	-4.928680000	0.878117000	0.498219000
6	-4.912380000	0.449049000	3.876259000
1	-3.777496000	1.642776000	5.273136000
1	-5.899816000	-0.587888000	2.258413000
1	-5.371828000	-0.165134000	4.655537000
6	-3.340890000	3.045473000	0.839335000
1	-3.845122000	4.017302000	0.980647000
1	-3.634816000	2.680891000	-0.160930000
6	3.431864000	3.682271000	-0.841612000
6	4.520315000	2.881082000	-1.230290000
6	3.639282000	5.054815000	-0.612932000
6	5.781835000	3.438451000	-1.383065000
1	4.351771000	1.813040000	-1.411392000
6	4.904110000	5.602143000	-0.773721000
1	2.795654000	5.679934000	-0.310170000
6	5.977099000	4.799215000	-1.156476000
1	6.621204000	2.807446000	-1.685992000
1	5.056338000	6.669949000	-0.596646000
1	6.970795000	5.237124000	-1.280192000
6	-1.759121000	0.272391000	-0.190424000
7	-1.882150000	-0.738104000	0.723573000
7	-2.718454000	-0.019164000	-1.127881000
6	-2.879694000	-1.642192000	0.355999000
6	-3.410311000	-1.187287000	-0.800358000
17	-3.313396000	-3.071181000	1.141626000
17	-4.659026000	-1.912625000	-1.673157000
6	-1.054090000	-0.930000000	1.895708000
17	-2.066445000	-1.128668000	3.329676000
17	-0.057008000	-2.398745000	1.626794000
17	0.030746000	0.432629000	2.197908000
6	-2.985946000	0.724357000	-2.343381000
17	-4.689872000	1.276464000	-2.339195000
17	-1.951602000	2.152017000	-2.481315000
17	-2.711586000	-0.318927000	-3.755148000
29	1.656436000	0.907399000	-0.513417000
6	2.216353000	-0.892905000	-0.383930000
7	1.795922000	-1.939620000	-1.159237000
7	2.958881000	-1.485985000	0.598043000
6	3.651791000	-0.807128000	1.683908000

17	3.499994000	0.948513000	1.582849000
17	5.380900000	-1.217007000	1.602966000
17	2.958486000	-1.345065000	3.234221000
6	2.962678000	-2.875362000	0.460541000
17	3.698460000	-4.001609000	1.477410000
6	2.223571000	-3.161124000	-0.636384000
17	1.835534000	-4.704459000	-1.198001000
6	0.929508000	-1.838957000	-2.314885000
17	1.656500000	-2.689844000	-3.689487000
17	-0.652322000	-2.573193000	-1.891372000
17	0.638073000	-0.164974000	-2.803302000

TS1<sub>Bi</sub>\_NHC-Cl

29	-0.363897000	1.665687000	-0.529474000
6	2.073176000	3.329259000	-0.863110000
6	1.359971000	2.285036000	-0.957424000
7	0.837458000	4.762814000	-0.264289000
7	-1.016145000	3.427544000	-0.010181000
7	-0.260602000	4.445050000	-0.032054000
6	-2.825524000	3.018722000	1.641664000
6	-2.145093000	3.375696000	2.810045000
6	-3.960851000	2.208176000	1.738961000
6	-2.638895000	2.996489000	4.053846000
1	-1.245087000	3.997261000	2.740608000
6	-4.448104000	1.815417000	2.984112000
1	-4.497102000	1.924843000	0.823246000
6	-3.801267000	2.232215000	4.144071000
1	-2.119906000	3.311419000	4.963367000
1	-5.351314000	1.201820000	3.048425000
1	-4.197827000	1.951936000	5.123848000
6	-2.424912000	3.603822000	0.311389000
1	-2.675858000	4.677546000	0.281861000
1	-3.018911000	3.126970000	-0.489697000
6	3.367254000	3.946215000	-0.971390000
6	4.377448000	3.182530000	-1.593681000
6	3.691474000	5.215157000	-0.471449000
6	5.669130000	3.673263000	-1.702538000
1	4.116092000	2.200459000	-2.004429000
6	4.989611000	5.697901000	-0.588615000
1	2.923394000	5.819853000	0.011002000
6	5.980897000	4.935285000	-1.199195000
1	6.438647000	3.070689000	-2.192085000
1	5.229921000	6.688745000	-0.194529000
1	6.997941000	5.325489000	-1.287812000
6	-1.742885000	0.381836000	-0.119240000
7	-1.860483000	-0.386478000	1.003713000
7	-2.876376000	0.106018000	-0.831927000
6	-3.037813000	-1.135029000	0.983120000
6	-3.683741000	-0.814898000	-0.161630000

17	-3.525979000	-2.308146000	2.092469000
17	-5.162709000	-1.441189000	-0.676509000
6	-0.892007000	-0.484836000	2.080655000
17	-1.686473000	-0.237366000	3.635808000
17	-0.157215000	-2.125042000	2.008185000
17	0.404598000	0.705591000	1.950710000
6	-3.212064000	0.625296000	-2.146204000
17	-4.765374000	1.499437000	-2.054664000
17	-1.983415000	1.747837000	-2.746754000
17	-3.350945000	-0.726966000	-3.292111000
29	1.644756000	0.387002000	-0.990778000
6	1.943547000	-1.461154000	-0.596390000
7	1.248990000	-2.553871000	-1.024419000
7	2.773925000	-1.949234000	0.367273000
6	3.744040000	-1.176412000	1.131790000
17	3.807115000	0.516503000	0.602801000
17	5.354393000	-1.885510000	0.894784000
17	3.285737000	-1.217026000	2.847331000
6	2.563658000	-3.312606000	0.573991000
17	3.324518000	-4.302062000	1.705988000
6	1.595526000	-3.691379000	-0.294317000
17	0.890809000	-5.220269000	-0.392937000
6	0.216868000	-2.549974000	-2.043076000
17	0.564701000	-3.794696000	-3.253794000
17	-1.355237000	-2.872648000	-1.247479000
17	0.106716000	-0.995156000	-2.877687000

TS1'<sub>Bi</sub>\_NHC-Cl

29	-0.962368000	-0.766922000	0.961073000
6	-3.356256000	0.954960000	0.552522000
6	-2.146500000	0.596889000	0.379535000
7	-4.187982000	-0.173293000	1.958203000
7	-2.255407000	-1.353866000	2.345128000
7	-3.372250000	-1.011565000	2.376815000
6	-4.470296000	1.782997000	0.156552000
6	-5.235571000	2.491396000	1.093890000
6	-4.800546000	1.868898000	-1.205738000
6	-6.318445000	3.255788000	0.677177000
1	-4.967791000	2.430396000	2.153677000
6	-5.883277000	2.635431000	-1.613966000
1	-4.208623000	1.300854000	-1.930058000
6	-6.649320000	3.323995000	-0.675045000
1	-6.908216000	3.808758000	1.413263000
1	-6.139659000	2.688430000	-2.675512000
1	-7.505082000	3.922203000	-0.998774000
6	0.664049000	-1.837845000	0.927032000
7	1.867425000	-1.584438000	1.521590000
7	0.849168000	-3.043745000	0.313900000
6	2.784805000	-2.608402000	1.273941000

6	2.138077000	-3.534426000	0.530690000
17	4.414526000	-2.652158000	1.708399000
17	2.795599000	-4.977346000	-0.042707000
6	2.219427000	-0.390806000	2.267008000
17	2.864311000	-0.844450000	3.853899000
17	3.454510000	0.503060000	1.318888000
17	0.843766000	0.683963000	2.524681000
6	-0.139696000	-3.780260000	-0.459085000
17	-0.456948000	-5.330996000	0.344403000
17	-1.666774000	-2.893310000	-0.595448000
17	0.488102000	-4.047913000	-2.103058000
29	-0.526391000	1.239887000	-0.395380000
6	1.222513000	1.800782000	-0.905624000
7	2.121143000	1.162997000	-1.712871000
7	1.914655000	2.873894000	-0.423873000
6	1.397362000	3.892351000	0.478726000
17	-0.306497000	3.616891000	0.872379000
17	1.537842000	5.478869000	-0.306082000
17	2.334592000	3.857362000	1.989932000
6	3.227832000	2.884570000	-0.894018000
17	4.438851000	3.993935000	-0.514943000
6	3.361381000	1.802894000	-1.696830000
17	4.780688000	1.298045000	-2.455428000
6	1.879273000	-0.060106000	-2.453426000
17	2.292351000	0.183247000	-4.160021000
17	2.894708000	-1.353297000	-1.740948000
17	0.193871000	-0.580954000	-2.367891000
6	-6.050490000	-0.772214000	0.474514000
6	-5.238352000	-1.501740000	-0.397600000
6	-7.255312000	-0.247304000	0.009125000
6	-5.623724000	-1.695804000	-1.718894000
1	-4.281104000	-1.900510000	-0.037493000
6	-7.646500000	-0.448381000	-1.311118000
1	-7.881132000	0.347186000	0.684427000
6	-6.828367000	-1.166032000	-2.178893000
1	-4.983283000	-2.266041000	-2.397396000
1	-8.590572000	-0.028647000	-1.668576000
1	-7.130585000	-1.317180000	-3.218507000
6	-5.613215000	-0.515410000	1.892400000
1	-5.784800000	-1.393281000	2.536212000
1	-6.195004000	0.314547000	2.321211000

IC<sub>Bi</sub>\_NHC-Cl

29	-0.407123000	1.627448000	-0.562145000
6	1.753083000	3.534007000	-0.805027000
6	1.235719000	2.324948000	-0.970931000
7	0.937223000	4.618072000	-0.338767000
7	-0.948120000	3.397572000	-0.114424000
7	-0.258652000	4.484788000	-0.062590000

6	-2.737079000	3.006010000	1.580509000
6	-2.028246000	3.405315000	2.718002000
6	-3.884643000	2.221384000	1.736969000
6	-2.503890000	3.090640000	3.986948000
1	-1.123530000	4.012570000	2.599161000
6	-4.357109000	1.899168000	3.007684000
1	-4.443985000	1.907493000	0.844944000
6	-3.679053000	2.355286000	4.134767000
1	-1.962627000	3.438562000	4.871193000
1	-5.271942000	1.309709000	3.117551000
1	-4.062189000	2.129572000	5.133805000
6	-2.359468000	3.533040000	0.220088000
1	-2.623473000	4.602436000	0.151909000
1	-2.959630000	3.017563000	-0.550862000
6	3.163602000	3.900344000	-1.007951000
6	4.013087000	3.049361000	-1.733224000
6	3.686894000	5.076849000	-0.460700000
6	5.358686000	3.353267000	-1.885461000
1	3.591177000	2.156937000	-2.213729000
6	5.034846000	5.379732000	-0.620388000
1	3.023144000	5.746064000	0.091833000
6	5.874581000	4.521035000	-1.325164000
1	6.007242000	2.688206000	-2.461744000
1	5.435516000	6.300467000	-0.188106000
1	6.932150000	4.767466000	-1.450066000
6	-1.785483000	0.335883000	-0.107007000
7	-1.871822000	-0.418287000	1.026945000
7	-2.917401000	0.028208000	-0.803679000
6	-3.035629000	-1.186896000	1.032212000
6	-3.702104000	-0.893431000	-0.109099000
17	-3.485986000	-2.357287000	2.159485000
17	-5.177704000	-1.549101000	-0.593541000
6	-0.894133000	-0.476348000	2.101444000
17	-1.683586000	-0.217434000	3.654861000
17	-0.121773000	-2.101631000	2.050159000
17	0.377774000	0.735308000	1.940598000
6	-3.280440000	0.521873000	-2.124127000
17	-4.835880000	1.383619000	-2.015061000
17	-2.073149000	1.640457000	-2.772808000
17	-3.421185000	-0.856656000	-3.238678000
29	1.693273000	0.486500000	-0.994379000
6	1.956793000	-1.382736000	-0.592148000
7	1.271048000	-2.491686000	-0.986275000
7	2.809930000	-1.840468000	0.365731000
6	3.785065000	-1.037698000	1.090268000
17	3.831841000	0.636691000	0.477721000
17	5.397252000	-1.738972000	0.857980000
17	3.348883000	-1.010317000	2.807912000
6	2.623126000	-3.200936000	0.604142000
17	3.404074000	-4.147372000	1.757628000

6	1.649144000	-3.610975000	-0.243479000
17	0.972206000	-5.153276000	-0.305622000
6	0.233131000	-2.532626000	-2.000739000
17	0.620515000	-3.779619000	-3.197038000
17	-1.322086000	-2.900536000	-1.193561000
17	0.067713000	-0.992576000	-2.847731000

TS2<sub>Bi</sub>\_NHC-Cl

29	0.559319000	-1.561478000	-0.580432000
6	-1.612661000	-3.567878000	-0.918872000
6	-0.949466000	-2.424435000	-1.082963000
7	-1.000089000	-4.700087000	-0.376890000
7	0.849916000	-3.455516000	-0.258541000
7	0.214732000	-4.572132000	-0.103790000
6	2.666678000	-3.090828000	1.428461000
6	1.967493000	-3.530768000	2.556547000
6	3.808482000	-2.301264000	1.604232000
6	2.441100000	-3.240922000	3.832207000
1	1.069345000	-4.144679000	2.424825000
6	4.283159000	-2.010970000	2.881487000
1	4.360407000	-1.954914000	0.720232000
6	3.610564000	-2.500712000	3.997372000
1	1.904359000	-3.616095000	4.707977000
1	5.194519000	-1.418690000	3.004417000
1	3.992254000	-2.296059000	5.001477000
6	2.284043000	-3.571044000	0.052183000
1	2.559924000	-4.633913000	-0.059600000
1	2.865680000	-3.017724000	-0.705100000
6	-3.053120000	-3.645246000	-1.206187000
6	-3.617867000	-2.852917000	-2.219420000
6	-3.884337000	-4.435999000	-0.405108000
6	-4.995096000	-2.825683000	-2.402720000
1	-2.953991000	-2.290108000	-2.887708000
6	-5.261837000	-4.403295000	-0.594942000
1	-3.432490000	-5.065793000	0.366456000
6	-5.819924000	-3.594040000	-1.583442000
1	-5.428312000	-2.216435000	-3.200297000
1	-5.909355000	-5.018952000	0.035125000
1	-6.903198000	-3.577363000	-1.728597000
6	1.862561000	-0.255489000	-0.075479000
7	1.907879000	0.465442000	1.080942000
7	2.974572000	0.129245000	-0.762992000
6	3.032454000	1.290273000	1.111889000
6	3.714752000	1.063484000	-0.036254000
17	3.419918000	2.447209000	2.275993000
17	5.162210000	1.795557000	-0.493772000
6	0.914510000	0.446401000	2.142242000
17	1.692616000	0.183163000	3.701422000
17	0.063800000	2.032506000	2.124569000

17	-0.298213000	-0.818524000	1.928449000
6	3.364423000	-0.316964000	-2.092080000
17	4.939564000	-1.139876000	-1.985247000
17	2.198794000	-1.451560000	-2.795206000
17	3.470655000	1.093509000	-3.168389000
29	-1.601118000	-0.612681000	-1.082119000
6	-1.985057000	1.207837000	-0.565854000
7	-1.367758000	2.372036000	-0.918753000
7	-2.852708000	1.577390000	0.418259000
6	-3.765804000	0.693474000	1.132326000
17	-3.682768000	-0.969524000	0.511553000
17	-5.425669000	1.278713000	0.908365000
17	-3.328774000	0.685991000	2.853114000
6	-2.754449000	2.939801000	0.698307000
17	-3.594196000	3.802515000	1.876096000
6	-1.812452000	3.438825000	-0.136116000
17	-1.225594000	5.019276000	-0.137712000
6	-0.336305000	2.520120000	-1.928711000
17	-0.803746000	3.787167000	-3.074686000
17	1.196534000	2.952210000	-1.107065000
17	-0.067714000	1.030851000	-2.837924000

#### P<sub>Bi</sub>\_NHC-Cl

7	-0.129653000	1.803052000	-2.906024000
7	-0.282244000	3.005170000	-3.446910000
7	-0.545993000	3.838629000	-2.498558000
6	-0.240737000	1.827888000	-1.526789000
6	-0.524753000	3.189543000	-1.306245000
29	1.104129000	0.674426000	-0.650082000
6	0.478991000	0.748507000	-3.677233000
1	-0.076899000	-0.196935000	-3.533136000
1	0.384690000	1.031799000	-4.738564000
6	1.924272000	0.560259000	-3.270776000
6	2.537500000	-0.692987000	-3.344595000
6	2.668623000	1.656591000	-2.809764000
6	3.860834000	-0.856790000	-2.936692000
6	3.991232000	1.491642000	-2.413028000
6	4.587246000	0.231875000	-2.458914000
1	1.967229000	-1.553616000	-3.712996000
1	2.208503000	2.651680000	-2.769210000
1	4.329695000	-1.843692000	-2.998485000
1	4.560189000	2.360037000	-2.070866000
1	5.627694000	0.104470000	-2.143321000
6	-0.737865000	3.913782000	-0.056109000
6	-0.989915000	5.293235000	-0.091045000
6	-0.667083000	3.272521000	1.190193000
6	-1.161875000	6.006596000	1.088214000
6	-0.831595000	3.992571000	2.367007000
6	-1.079905000	5.362563000	2.320829000

1	-1.045230000	5.790943000	-1.062568000
1	-0.467696000	2.193889000	1.240219000
1	-1.359389000	7.080958000	1.045752000
1	-0.758892000	3.481916000	3.331362000
1	-1.209161000	5.928463000	3.246988000
6	3.799159000	1.277777000	1.247421000
7	3.550575000	-0.072330000	0.762178000
6	2.434402000	-0.491592000	0.099606000
7	2.606334000	-1.842141000	-0.023362000
6	1.646067000	-2.799380000	-0.548156000
6	3.813438000	-2.250057000	0.551947000
6	4.405608000	-1.138014000	1.044399000
29	-1.331454000	0.481287000	-0.612590000
6	-2.776832000	-0.483225000	0.191762000
7	-3.969290000	-0.752525000	-0.409154000
6	-4.213072000	-0.743381000	-1.842040000
6	-4.966817000	-1.007765000	0.533912000
6	-4.371294000	-0.950838000	1.748961000
7	-3.020530000	-0.681354000	1.517765000
6	-2.030362000	-0.573331000	2.576535000
17	0.219944000	-2.016506000	-1.256716000
17	2.399072000	-3.796648000	-1.814228000
17	1.095096000	-3.828724000	0.796880000
17	4.409468000	-3.822902000	0.680678000
17	5.867102000	-1.084013000	1.883260000
17	3.783911000	1.237922000	3.027420000
17	5.375039000	1.852395000	0.665924000
17	2.551181000	2.419823000	0.708734000
17	-0.380093000	-0.533675000	1.901670000
17	-2.123512000	-1.997310000	3.631704000
17	-2.332036000	0.917543000	3.485589000
17	-5.142738000	-1.057024000	3.243699000
17	-6.604848000	-1.262863000	0.232819000
17	-5.296084000	0.597776000	-2.239405000
17	-4.914819000	-2.299005000	-2.324958000
17	-2.692819000	-0.542263000	-2.756341000

AC<sub>Mo</sub>\_NHC-Br

6	3.546934000	-0.002329000	0.000857000
6	4.772110000	-0.002794000	0.137452000
29	1.701494000	-0.000727000	-0.216713000
6	6.181498000	-0.003504000	0.303736000
6	7.045049000	0.098420000	-0.804679000
6	6.758131000	-0.105970000	1.585135000
6	8.422859000	0.097543000	-0.634597000
6	8.136915000	-0.105405000	1.745897000
6	8.978061000	-0.003912000	0.639467000
1	6.608658000	0.178255000	-1.803820000
1	6.097175000	-0.185778000	2.452151000



1	9.074519000	0.177599000	-1.509573000
1	8.562951000	-0.185658000	2.750240000
1	10.063483000	-0.004007000	0.769806000
35	-0.830568000	-3.401568000	1.486397000
6	-0.631629000	-2.468849000	-0.211385000
35	-1.752178000	-3.298513000	-1.583008000
35	1.186736000	-2.703877000	-0.789288000
7	-1.019738000	-1.082667000	-0.051527000
6	-0.187914000	0.000364000	-0.192935000
7	-1.018642000	1.083626000	-0.046670000
6	-0.629093000	2.470099000	-0.200181000
35	1.189620000	2.706087000	-0.776403000
35	-1.748545000	3.307150000	-1.568390000
35	-0.827634000	3.395478000	1.501634000
35	-3.779077000	1.724530000	0.681913000
6	-2.320826000	0.677800000	0.263192000
6	-2.321551000	-0.676880000	0.260166000
35	-3.780774000	-1.723959000	0.674587000

TS1<sub>Mo</sub>\_NHC-Br

7	-1.938109000	-0.138579000	1.932451000
7	-3.116418000	-0.251894000	2.399684000
7	-4.189254000	-0.540034000	2.004319000
6	-3.260785000	-0.708977000	-0.351933000
6	-4.430685000	-0.775562000	0.134294000
29	-1.446944000	-0.463640000	-0.039634000
6	-0.971458000	0.549977000	2.769489000
1	-0.736547000	1.529354000	2.302969000
1	-1.424287000	0.769241000	3.752500000
6	0.313727000	-0.214429000	2.925340000
6	1.530118000	0.470049000	2.929686000
6	0.315686000	-1.605928000	3.048203000
6	2.733330000	-0.218191000	3.045303000
6	1.517048000	-2.295023000	3.172771000
6	2.729062000	-1.605587000	3.162622000
1	1.529856000	1.558669000	2.779147000
1	-0.636243000	-2.147305000	3.027876000
1	3.680581000	0.330435000	3.004402000
1	1.510747000	-3.385504000	3.259176000
1	3.673486000	-2.153788000	3.230107000
6	-5.843005000	-0.964672000	-0.092628000
6	-6.819190000	-0.841431000	0.906701000
6	-6.254435000	-1.283968000	-1.400998000
6	-8.162004000	-1.032120000	0.599988000
6	-7.595894000	-1.472082000	-1.696462000
6	-8.558621000	-1.347183000	-0.696004000
1	-6.518809000	-0.595240000	1.925278000
1	-5.492280000	-1.383879000	-2.179109000
1	-8.911088000	-0.932239000	1.390442000

1	-7.894605000	-1.720789000	-2.718516000
1	-9.616558000	-1.496153000	-0.927940000
35	1.627571000	-2.345795000	-2.618155000
6	1.342057000	-2.284429000	-0.676538000
35	2.526489000	-3.596237000	0.139555000
35	-0.467475000	-2.923481000	-0.295308000
7	1.495388000	-0.959796000	-0.211352000
6	0.424813000	-0.046808000	-0.127727000
7	0.917692000	1.160864000	-0.006185000
6	-0.610238000	3.302200000	-0.559193000
35	-1.995123000	2.146514000	-0.580792000
35	-0.073355000	4.105151000	1.004578000
35	0.352332000	3.628944000	-2.088688000
35	3.350886000	2.570928000	0.180782000
6	2.264389000	1.085693000	-0.073672000
6	2.674414000	-0.206073000	-0.224375000
35	4.409591000	-0.810422000	-0.350502000

TS1'<sub>Mo</sub>\_NHC-Br

7	-0.742505000	-0.700363000	-1.168056000
7	-1.751092000	-0.815028000	-1.779274000
7	-2.923429000	-1.254415000	-1.631902000
6	-2.305736000	-1.610206000	0.954278000
6	-3.342704000	-1.763200000	0.231377000
29	-0.607400000	-0.942237000	0.821031000
6	-4.756462000	-2.052484000	0.185920000
6	-5.609649000	-1.430942000	1.113802000
6	-5.316370000	-2.904040000	-0.777531000
6	-6.980900000	-1.638865000	1.060771000
6	-6.691249000	-3.103498000	-0.830169000
6	-7.529886000	-2.466821000	0.082880000
1	-5.169928000	-0.758768000	1.857128000
1	-4.650124000	-3.398496000	-1.491957000
1	-7.632099000	-1.137813000	1.782755000
1	-7.113807000	-3.768813000	-1.588840000
1	-8.611118000	-2.622786000	0.036646000
35	1.224502000	3.773066000	1.560674000
6	0.316937000	2.275155000	0.698138000
35	-0.557729000	2.864074000	-0.938587000
35	-1.055004000	1.699524000	1.929196000
7	1.268568000	1.236767000	0.392444000
6	1.121625000	-0.074159000	0.753381000
7	2.225128000	-0.695882000	0.244064000
6	2.472981000	-2.112325000	0.363813000
35	1.298901000	-2.968586000	1.636806000
35	2.210935000	-2.954694000	-1.366626000
35	4.284368000	-2.422265000	1.017197000
35	4.467673000	-0.182096000	-1.555792000
6	2.987738000	0.189572000	-0.523479000

6	2.391158000	1.403263000	-0.425705000
35	2.965873000	2.933840000	-1.275265000
6	-3.978888000	-0.592910000	-2.396656000
1	-3.521286000	-0.113662000	-3.277868000
1	-4.681538000	-1.349313000	-2.778671000
6	-4.724737000	0.415194000	-1.559120000
6	-4.042326000	1.193907000	-0.619139000
6	-6.108591000	0.540834000	-1.673509000
6	-4.737291000	2.086384000	0.188369000
6	-6.804748000	1.436775000	-0.867140000
6	-6.121211000	2.208723000	0.068305000
1	-2.960929000	1.067513000	-0.488206000
1	-6.650089000	-0.099898000	-2.379429000
1	-4.192299000	2.685980000	0.924597000
1	-7.891766000	1.517306000	-0.955655000
1	-6.668455000	2.903785000	0.711080000

AC<sub>Bi</sub>\_NHC-Br

6	0.000628000	-3.379155000	-0.001929000
6	0.001494000	-4.620533000	-0.001368000
29	1.071326000	-1.874151000	0.572720000
6	0.002446000	-6.036425000	-0.000793000
6	-0.416144000	-6.751477000	1.138807000
6	0.421978000	-6.751921000	-1.139760000
6	-0.409280000	-8.138165000	1.135227000
6	0.416956000	-8.138616000	-1.134946000
6	0.004304000	-8.834150000	0.000448000
1	-0.740290000	-6.197933000	2.023803000
1	0.745379000	-6.198738000	-2.025253000
1	-0.731693000	-8.684960000	2.024980000
1	0.740086000	-8.685770000	-2.024217000
1	0.005033000	-9.927283000	0.000929000
6	4.064571000	-0.644674000	-0.303518000
7	3.139553000	0.182050000	0.450403000
6	1.954538000	-0.237637000	0.984937000
7	1.484081000	0.842767000	1.676168000
6	0.269520000	0.876743000	2.466318000
6	2.331611000	1.943702000	1.513700000
6	3.376462000	1.524640000	0.754853000
29	-1.070926000	-1.874390000	-0.575290000
6	-1.954600000	-0.237641000	-0.985708000
7	-3.139805000	0.180917000	-0.450713000
6	-4.064422000	-0.647040000	0.302349000
6	-3.377366000	1.523714000	-0.753707000
6	-2.332743000	1.944086000	-1.512131000
7	-1.484672000	0.843729000	-1.675788000
6	-0.270067000	0.879198000	-2.465813000
35	1.021580000	2.063578000	-1.604116000
35	0.586632000	-0.843361000	-2.671080000

35	-0.669534000	1.491867000	-4.263061000
35	-3.457487000	-2.483178000	0.472869000
35	-5.769688000	-0.708424000	-0.622073000
35	-4.281294000	0.039773000	2.103754000
35	-4.762140000	2.590491000	-0.183666000
35	-2.060321000	3.683369000	-2.047179000
35	-0.586192000	-0.846523000	2.669813000
35	-1.022909000	2.061300000	1.605997000
35	0.668809000	1.487747000	4.264156000
35	2.058243000	3.682299000	2.050520000
35	4.760705000	2.592751000	0.185990000
35	4.281110000	0.044206000	-2.104190000
35	5.769841000	-0.706186000	0.620882000
35	3.458545000	-2.480901000	-0.475989000

TS1<sub>Bi</sub>\_NHC-Br

29	-0.855562000	1.997610000	-0.456538000
6	1.123568000	4.085314000	-1.201708000
6	0.629234000	2.918974000	-1.157977000
7	-0.228368000	5.296325000	-0.384864000
7	-1.731122000	3.647909000	0.174473000
7	-1.194213000	4.785101000	0.024274000
6	-3.233498000	3.055762000	2.079479000
6	-2.532617000	3.647029000	3.135515000
6	-4.183446000	2.069394000	2.363577000
6	-2.835293000	3.315581000	4.451568000
1	-1.774157000	4.408371000	2.918798000
6	-4.488246000	1.737433000	3.682159000
1	-4.730418000	1.597973000	1.536124000
6	-3.830812000	2.378442000	4.727989000
1	-2.305034000	3.807443000	5.271750000
1	-5.255122000	0.986780000	3.892536000
1	-4.087419000	2.142062000	5.764486000
6	-3.096265000	3.583400000	0.674250000
1	-3.556605000	4.584056000	0.609554000
1	-3.673752000	2.936788000	-0.010556000
6	2.237045000	4.926242000	-1.544858000
6	3.157250000	4.411860000	-2.483754000
6	2.489915000	6.179037000	-0.967266000
6	4.300008000	5.124584000	-2.817486000
1	2.940319000	3.448041000	-2.958354000
6	3.635284000	6.885732000	-1.313462000
1	1.784865000	6.591333000	-0.244341000
6	4.543440000	6.365614000	-2.232311000
1	5.000162000	4.714590000	-3.550124000
1	3.822304000	7.860699000	-0.855804000
1	5.439944000	6.931285000	-2.498333000
6	-1.900590000	0.500883000	0.152681000
7	-1.699024000	-0.239841000	1.285303000

7	-3.029255000	-0.031629000	-0.415495000
6	-2.672852000	-1.234553000	1.407661000
6	-3.520086000	-1.089747000	0.357594000
35	-2.727999000	-2.637382000	2.598363000
35	-4.984451000	-2.157155000	0.041223000
6	-0.640422000	-0.047385000	2.263354000
35	-1.388438000	0.107572000	4.037977000
35	0.603767000	-1.560243000	2.175269000
35	0.409289000	1.551088000	2.005866000
6	-3.652951000	0.394927000	-1.656528000
35	-5.469566000	1.011935000	-1.302301000
35	-2.724341000	1.851432000	-2.526555000
35	-3.710636000	-1.064373000	-2.941715000
29	1.344463000	1.121075000	-1.164342000
6	2.190958000	-0.579020000	-0.850421000
7	1.708542000	-1.824486000	-1.130768000
7	3.254219000	-0.798144000	-0.024848000
6	4.167042000	0.224423000	0.457984000
35	3.823213000	1.968850000	-0.325262000
35	5.982755000	-0.243880000	-0.051703000
35	4.015129000	0.396263000	2.382506000
6	3.372622000	-2.155024000	0.285103000
35	4.510743000	-2.948730000	1.490712000
6	2.398273000	-2.800284000	-0.406700000
35	2.000662000	-4.589102000	-0.249563000
6	0.623369000	-2.110543000	-2.043787000
35	1.192941000	-3.413201000	-3.363415000
35	-0.912162000	-2.774146000	-1.041159000
35	0.035258000	-0.556823000	-3.037178000

TS1'Bi\_NHC-Br

29	-0.463088000	-2.009953000	0.566795000
6	-3.425308000	-2.021839000	0.264466000
6	-2.226925000	-1.716263000	-0.031632000
7	-3.421100000	-3.478687000	1.620596000
7	-1.138162000	-3.431657000	1.832989000
7	-2.254566000	-3.761067000	1.941346000
6	-4.829531000	-1.730345000	0.121904000
6	-5.644955000	-1.495909000	1.241566000
6	-5.384446000	-1.632279000	-1.165206000
6	-6.989446000	-1.188818000	1.073713000
1	-5.204729000	-1.560862000	2.242092000
6	-6.729947000	-1.325607000	-1.322007000
1	-4.745696000	-1.827179000	-2.032423000
6	-7.536769000	-1.110891000	-0.206005000
1	-7.617551000	-1.005052000	1.949595000
1	-7.156965000	-1.262317000	-2.326467000
1	-8.596502000	-0.875290000	-0.333660000
6	1.389507000	-1.524782000	0.879624000

7	1.893821000	-0.524127000	1.664993000
7	2.492330000	-2.116030000	0.326481000
6	3.290922000	-0.487413000	1.589675000
6	3.666247000	-1.498644000	0.768209000
35	4.445021000	0.761192000	2.295655000
35	5.406738000	-1.889854000	0.319956000
6	1.128371000	0.394414000	2.490049000
35	1.752526000	0.301295000	4.327285000
35	1.326040000	2.208238000	1.780034000
35	-0.763550000	0.035139000	2.550674000
6	2.492104000	-3.279860000	-0.542537000
35	3.377480000	-4.749954000	0.363742000
35	0.711282000	-3.885582000	-1.007141000
35	3.378713000	-2.879575000	-2.226470000
29	-1.480638000	-0.083757000	-0.726449000
6	-0.823527000	1.688356000	-1.016196000
7	0.356495000	2.049184000	-1.604194000
7	-1.300249000	2.842925000	-0.463439000
6	-2.594738000	3.005976000	0.180651000
35	-3.682233000	1.404947000	0.146173000
35	-3.601733000	4.375919000	-0.765094000
35	-2.353127000	3.494123000	2.045032000
6	-0.391004000	3.890204000	-0.637278000
35	-0.477139000	5.600559000	0.033416000
6	0.651817000	3.390706000	-1.348352000
35	2.195519000	4.310347000	-1.743243000
6	1.201432000	1.177505000	-2.390471000
35	1.510812000	1.956638000	-4.140516000
35	2.888864000	0.889653000	-1.455179000
35	0.426967000	-0.569116000	-2.704402000
6	-5.098851000	-4.725616000	0.341617000
6	-4.271378000	-4.963342000	-0.758590000
6	-6.481825000	-4.699282000	0.164263000
6	-4.821890000	-5.165024000	-2.019011000
1	-3.183025000	-4.965965000	-0.626564000
6	-7.034432000	-4.908743000	-1.095661000
1	-7.131242000	-4.490261000	1.021980000
6	-6.205084000	-5.135557000	-2.190290000
1	-4.168963000	-5.349484000	-2.876425000
1	-8.119737000	-4.882498000	-1.224883000
1	-6.637109000	-5.293327000	-3.182029000
6	-4.505359000	-4.457415000	1.700240000
1	-4.110531000	-5.379506000	2.157215000
1	-5.286074000	-4.070535000	2.376439000

AC<sub>Mo</sub>\_NHC-I

6	3.440025000	0.609860000	-0.012265000
6	4.551686000	0.752974000	-0.525059000
29	1.761080000	0.356064000	0.728500000

6	5.830216000	0.915294000	-1.117098000
6	7.002892000	0.548550000	-0.427383000
6	5.963996000	1.445646000	-2.415770000
6	8.250961000	0.706400000	-1.013920000
6	7.215968000	1.598969000	-2.995127000
6	8.366399000	1.231303000	-2.299770000
1	6.910285000	0.136016000	0.580659000
1	5.060201000	1.733735000	-2.959008000
1	9.148345000	0.415099000	-0.460354000
1	7.296900000	2.012180000	-4.004742000
1	9.351005000	1.353661000	-2.758860000
53	-0.037458000	3.307815000	-1.289811000
6	-0.802479000	2.333539000	0.508015000
53	-2.596123000	3.316906000	1.282268000
53	0.682917000	2.618479000	2.135193000
7	-1.020904000	0.934463000	0.242923000
6	-0.104169000	0.003666000	0.618299000
7	-0.620653000	-1.197586000	0.245463000
6	0.091725000	-2.421895000	0.511378000
53	1.564191000	-2.149859000	2.149948000
53	-1.223741000	-3.992633000	1.275453000
53	1.170369000	-3.039720000	-1.281770000
53	-2.767604000	-2.395929000	-1.699010000
6	-1.763574000	-1.004436000	-0.540723000
6	-2.016280000	0.338387000	-0.541535000
53	-3.462577000	1.269201000	-1.693728000

TS1<sub>Mo</sub>\_NHC-I

7	2.457693000	-0.203175000	2.081530000
7	3.671695000	-0.292048000	2.469153000
7	4.749152000	-0.097419000	2.035270000
6	3.767808000	0.472123000	-0.241330000
6	4.966381000	0.409082000	0.166303000
29	1.949236000	0.276391000	0.200563000
6	1.466233000	-0.803029000	2.954042000
1	1.141865000	-1.777541000	2.531927000
1	1.919693000	-1.031819000	3.935098000
6	0.261678000	0.082441000	3.120574000
6	-1.025537000	-0.458759000	3.145179000
6	0.415592000	1.466068000	3.251161000
6	-2.141520000	0.362803000	3.288885000
6	-0.695905000	2.287160000	3.393026000
6	-1.980017000	1.739756000	3.402766000
1	-1.158157000	-1.542187000	3.025661000
1	1.422767000	1.894754000	3.224832000
1	-3.145652000	-0.077022000	3.282986000
1	-0.562642000	3.369091000	3.488181000
1	-2.854911000	2.391213000	3.494472000
6	6.383667000	0.480043000	-0.076199000

6	7.347828000	0.541141000	0.941506000
6	6.819591000	0.503028000	-1.415355000
6	8.699220000	0.620249000	0.623519000
6	8.169810000	0.581622000	-1.721910000
6	9.119374000	0.639361000	-0.703013000
1	7.028666000	0.528939000	1.984001000
1	6.069821000	0.456114000	-2.210273000
1	9.436855000	0.668828000	1.429634000
1	8.486032000	0.596142000	-2.768732000
1	10.184022000	0.699972000	-0.943994000
53	-0.958223000	2.350157000	-2.620482000
6	-0.630089000	2.369566000	-0.425556000
53	-1.805015000	4.034412000	0.425615000
53	1.403733000	3.040340000	-0.022315000
7	-0.910073000	1.025718000	0.040524000
6	0.066517000	0.039938000	0.005068000
7	-0.623125000	-1.155156000	0.032109000
6	-0.077825000	-2.442397000	-0.333722000
53	2.064077000	-2.512629000	-0.672935000
53	-0.416828000	-4.016394000	1.189814000
53	-0.988270000	-3.064199000	-2.264541000
53	-3.546348000	-2.258993000	0.434606000
6	-2.006267000	-0.910363000	0.082945000
6	-2.181629000	0.434885000	0.042389000
53	-4.062241000	1.302295000	-0.052817000

TS1'<sub>Mo</sub>\_NHC-I

7	-1.082417000	-0.375445000	-0.959871000
7	-2.013100000	-0.626509000	-1.648839000
7	-3.148577000	-1.164915000	-1.551261000
6	-2.749349000	-1.189027000	1.095400000
6	-3.682121000	-1.518521000	0.289136000
29	-1.027526000	-0.555669000	1.063669000
6	-5.035723000	-2.009180000	0.156353000
6	-6.061366000	-1.418818000	0.913028000
6	-5.364133000	-3.040336000	-0.735794000
6	-7.377194000	-1.834078000	0.760078000
6	-6.683957000	-3.449315000	-0.887539000
6	-7.696882000	-2.843174000	-0.146963000
1	-5.802689000	-0.608483000	1.601339000
1	-4.561534000	-3.509661000	-1.313895000
1	-8.166429000	-1.355669000	1.347105000
1	-6.925180000	-4.254449000	-1.587778000
1	-8.735031000	-3.162863000	-0.271603000
53	1.816122000	3.990997000	1.360231000
6	0.381284000	2.427108000	0.785787000
53	-1.038558000	3.171302000	-0.705592000
53	-0.765323000	2.028825000	2.616435000
7	1.063896000	1.257089000	0.316261000



6	0.825099000	0.023951000	0.844845000
7	1.662907000	-0.825141000	0.189102000
6	1.733396000	-2.221099000	0.525190000
53	0.768383000	-2.652239000	2.456852000
53	0.739786000	-3.438513000	-0.989319000
53	3.819312000	-2.852458000	0.825101000
53	3.451236000	-0.965358000	-2.382053000
6	2.303854000	-0.158208000	-0.859262000
6	1.935448000	1.153907000	-0.773120000
53	2.538773000	2.639356000	-2.083429000
6	-4.170972000	-0.777041000	-2.518042000
1	-3.668958000	-0.316306000	-3.384559000
1	-4.681654000	-1.679131000	-2.891452000
6	-5.188397000	0.162813000	-1.921951000
6	-4.797658000	1.159026000	-1.022129000
6	-6.540530000	0.011381000	-2.228336000
6	-5.750717000	1.988578000	-0.441642000
6	-7.493527000	0.845431000	-1.652059000
6	-7.100524000	1.833431000	-0.753565000
1	-3.741653000	1.252358000	-0.737013000
1	-6.851079000	-0.795066000	-2.902946000
1	-5.437714000	2.756072000	0.271928000
1	-8.552120000	0.709046000	-1.890158000
1	-7.848681000	2.480692000	-0.287648000

#### AC<sub>Bi</sub>\_NHC-I

6	-0.029024000	-3.322590000	-0.521102000
6	0.736962000	-4.278227000	-0.327238000
29	1.180989000	-1.880805000	0.165362000
6	1.730303000	-5.273789000	-0.144887000
6	2.021117000	-5.782508000	1.134217000
6	2.521172000	-5.684427000	-1.240009000
6	3.075022000	-6.667145000	1.311811000
6	3.577067000	-6.568515000	-1.048883000
6	3.856644000	-7.058534000	0.225063000
1	1.409596000	-5.465425000	1.983582000
1	2.282084000	-5.303774000	-2.238103000
1	3.294404000	-7.055895000	2.309479000
1	4.182757000	-6.883211000	-1.902780000
1	4.686998000	-7.753844000	0.372267000
6	4.189723000	-0.493060000	-0.691784000
7	3.265093000	0.207666000	0.177457000
6	2.196154000	-0.381334000	0.785973000
7	1.747101000	0.531698000	1.695606000
6	0.740142000	0.240655000	2.688585000
6	2.431918000	1.744135000	1.548874000
6	3.392834000	1.536850000	0.601532000
29	-1.245869000	-1.966322000	-0.977024000
6	-2.369650000	-0.421356000	-1.102528000

7	-3.530047000	-0.306497000	-0.406088000
6	-4.299637000	-1.461557000	0.008132000
6	-3.834756000	1.041196000	-0.190457000
6	-2.912116000	1.766960000	-0.890111000
7	-2.041838000	0.841559000	-1.485060000
6	-0.980691000	1.138712000	-2.417476000
53	0.648810000	2.220937000	-1.440532000
53	-0.084464000	-0.668317000	-3.300645000
53	-1.773610000	2.248102000	-4.128659000
53	-3.751060000	-3.253795000	-1.169421000
53	-6.424157000	-1.208768000	-0.431328000
53	-3.942427000	-1.901616000	2.107854000
53	-5.109868000	1.821293000	1.242423000
53	-2.764194000	3.829532000	-0.851345000
53	0.314131000	-1.913039000	2.892897000
53	-1.158409000	1.212310000	2.175176000
53	1.418333000	0.811024000	4.690853000
53	1.911757000	3.602012000	2.307009000
53	4.588278000	3.028728000	-0.195848000
53	4.089999000	0.238341000	-2.747977000
53	6.222856000	-0.340688000	0.118773000
53	3.808068000	-2.657092000	-0.802022000

TS1<sub>Bi</sub>\_NHC-I

29	-1.078239000	2.105074000	-0.370115000
6	0.691023000	4.250943000	-1.432558000
6	0.324935000	3.055993000	-1.215041000
7	-0.644071000	5.459332000	-0.607905000
7	-2.021861000	3.796162000	0.186450000
7	-1.555934000	4.936419000	-0.099018000
6	-3.506252000	3.462577000	2.179693000
6	-2.744830000	4.176243000	3.110745000
6	-4.509010000	2.603590000	2.637746000
6	-3.017155000	4.070349000	4.469605000
1	-1.948968000	4.842234000	2.757671000
6	-4.794063000	2.509706000	3.997964000
1	-5.102337000	2.035898000	1.909761000
6	-4.056616000	3.252726000	4.914785000
1	-2.428354000	4.646037000	5.188996000
1	-5.599649000	1.855050000	4.341766000
1	-4.288757000	3.195626000	5.981991000
6	-3.380043000	3.729001000	0.702697000
1	-3.912797000	4.663369000	0.452498000
1	-3.902517000	2.927930000	0.151096000
6	1.702212000	5.124612000	-1.955757000
6	2.480611000	4.647859000	-3.034784000
6	2.017379000	6.371916000	-1.396103000
6	3.559465000	5.386416000	-3.510378000
1	2.203016000	3.696942000	-3.503896000

6	3.092059000	7.103497000	-1.885407000
1	1.416805000	6.754885000	-0.569434000
6	3.870208000	6.615315000	-2.933993000
1	4.149520000	5.005529000	-4.348428000
1	3.330449000	8.071806000	-1.437418000
1	4.714215000	7.199399000	-3.309262000
6	-2.095758000	0.601283000	0.266271000
7	-1.851383000	-0.109475000	1.412644000
7	-3.184008000	-0.008591000	-0.315654000
6	-2.751460000	-1.177562000	1.527148000
6	-3.601147000	-1.099442000	0.464639000
53	-2.702877000	-2.784490000	2.839427000
53	-5.151059000	-2.441078000	0.149217000
6	-0.847591000	0.196496000	2.418343000
53	-1.784467000	0.424941000	4.381081000
53	0.746967000	-1.340562000	2.435383000
53	0.251689000	2.065345000	2.177151000
6	-3.857926000	0.403388000	-1.535397000
53	-5.920797000	1.036499000	-1.074768000
53	-2.963103000	2.091184000	-2.596490000
53	-3.915528000	-1.174125000	-3.077409000
29	1.257665000	1.332341000	-1.163869000
6	2.309112000	-0.275848000	-0.846487000
7	1.938660000	-1.569487000	-1.071965000
7	3.420037000	-0.353023000	-0.057578000
6	4.302559000	0.764271000	0.208150000
53	3.786944000	2.543476000	-0.984564000
53	6.344048000	0.272781000	-0.439114000
53	4.263120000	1.348260000	2.308481000
6	3.650900000	-1.677581000	0.332133000
53	4.929137000	-2.372235000	1.804894000
6	2.724517000	-2.444845000	-0.310164000
53	2.445430000	-4.469069000	0.026209000
6	0.936224000	-1.966171000	-2.028334000
53	1.777272000	-3.366078000	-3.487245000
53	-0.818733000	-2.817446000	-1.026479000
53	0.192330000	-0.295657000	-3.249579000

TS1'Bi\_NHC-I

29	-0.892891000	1.824971000	1.002774000
6	1.179475000	3.990388000	0.821736000
6	0.632390000	2.863286000	0.588885000
7	0.112697000	5.054834000	2.085250000
7	-1.432403000	3.372820000	2.317123000
7	-0.914236000	4.414241000	2.395274000
6	2.306026000	4.843104000	0.551190000
6	2.709840000	5.017429000	-0.787007000
6	3.049017000	5.452192000	1.573191000
6	3.828662000	5.789346000	-1.087245000

1	2.108968000	4.557787000	-1.581002000
6	4.160453000	6.225381000	1.263082000
1	2.745837000	5.297022000	2.613350000
6	4.551654000	6.399830000	-0.064560000
1	4.128336000	5.927289000	-2.129846000
1	4.737554000	6.691309000	2.066484000
1	5.426699000	7.010429000	-0.301327000
6	-2.156254000	0.355114000	0.987472000
7	-2.001457000	-0.843754000	1.633786000
7	-3.301743000	0.215274000	0.244769000
6	-2.998337000	-1.746488000	1.243278000
6	-3.840641000	-1.070124000	0.412817000
53	-3.051638000	-3.808315000	1.494806000
53	-5.574059000	-1.901012000	-0.365440000
6	-0.992622000	-1.145053000	2.631554000
53	-1.918513000	-1.984700000	4.443171000
53	0.542743000	-2.490146000	1.799546000
53	0.095488000	0.573093000	3.411272000
6	-3.953428000	1.259593000	-0.524386000
53	-5.825231000	1.811276000	0.476975000
53	-2.827586000	3.122725000	-0.720765000
53	-4.310861000	0.684802000	-2.621014000
29	1.331492000	1.326033000	-0.348860000
6	2.123432000	-0.328751000	-0.952621000
7	1.541167000	-1.342699000	-1.652794000
7	3.239179000	-0.869275000	-0.391650000
6	4.265255000	-0.067070000	0.242684000
53	4.075774000	2.075405000	-0.282506000
53	6.252028000	-0.606343000	-0.499548000
53	4.129956000	-0.231656000	2.408987000
6	3.256284000	-2.254530000	-0.580947000
53	4.361718000	-3.652429000	0.473158000
6	2.203388000	-2.552238000	-1.397182000
53	1.651584000	-4.469312000	-1.946405000
6	0.446560000	-1.150776000	-2.568175000
53	1.001486000	-1.830433000	-4.571612000
53	-1.360171000	-2.153444000	-1.849324000
53	-0.098074000	0.966981000	-2.815767000
6	0.075075000	6.514809000	1.974644000
1	0.908390000	6.935579000	2.559927000
1	-0.857015000	6.874651000	2.439731000
6	0.184937000	6.962179000	0.539582000
6	1.095745000	7.952890000	0.174659000
6	-0.588335000	6.351184000	-0.449349000
6	1.236018000	8.323444000	-1.159670000
6	-0.446245000	6.712159000	-1.783652000
6	0.472303000	7.698412000	-2.141422000
1	1.719583000	8.420783000	0.944739000
1	-1.297829000	5.566863000	-0.153854000
1	1.956686000	9.097774000	-1.435890000

1	-1.056530000	6.229362000	-2.552349000
1	0.587466000	7.983573000	-3.190402000