

Metallo phosphonate catalyzed benzoin couplings: The influence of the counterion

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Table S1. Cartesien coordinates of benzoylsilane

C	-4.01058900	0.85450100	0.76120700
C	-2.68002200	0.67058600	1.13358900
5 C	-1.64566700	0.93128100	0.22356800
C	-1.96428900	1.38300100	-1.06002500
C	-3.29853500	1.56733200	-1.43054400
C	-4.32508200	1.30268900	-0.52401800
H	-4.80249200	0.64874600	1.47661900
10 H	-2.43924300	0.32434600	2.13548400
H	-1.16357000	1.59518300	-1.75997500
H	-3.53354700	1.92116000	-2.43125100
H	-5.36244200	1.44679500	-0.81411300
C	-0.19546400	0.74450500	0.66644500
15 H	-0.01931000	1.40553900	1.52654700
C	0.02087400	-0.67633200	1.24886900
C	0.17272800	-1.87111900	0.36304000
C	0.03502800	-1.82523400	-1.03403200
C	0.44229600	-3.10263100	0.98472600
20 C	0.16100100	-2.99177000	-1.78783800
H	-0.16659800	-0.88344800	-1.52775700
C	0.57402900	-4.26273800	0.22915400
H	0.53943200	-3.12183900	2.06523700
C	0.43201300	-4.20930100	-1.16092000
25 H	0.04783900	-2.94895200	-2.86769300
H	0.78374400	-5.20938900	0.71981700
H	0.53177800	-5.11536000	-1.75309400
O	0.03911200	-0.78885300	2.46771400
O	0.70437700	1.03987900	-0.38689300
30 Si	2.24286900	1.70832200	-0.15865600
C	3.31521700	0.54836400	0.87133300
H	3.43119400	-0.42503500	0.38084600
H	4.31724500	0.97110100	1.01733000
H	2.88530700	0.36950300	1.86397700
35 C	2.08373100	3.38193600	0.69988700
H	3.06962400	3.84661300	0.82657500
H	1.46281900	4.07071400	0.11539600
H	1.63662200	3.29469900	1.69727700
C	2.92193300	1.89944600	-1.90055700
40 H	2.28759400	2.55806200	-2.50470500
H	3.93094500	2.32911900	-1.88560900
H	2.97977100	0.93063200	-2.40959400

45 Table S2. Cartesien coordinates of benzaldehyde

C	1.73604900	1.06060300	-0.00000900
C	0.36121100	1.29213000	0.00002500
C	-0.53386900	0.21449000	0.00000900
50 C	-0.04508100	-1.10119100	0.00002000
C	1.32634800	-1.33130600	0.00001000
C	2.21688900	-0.25078300	-0.00002400
H	2.43035000	1.89611300	-0.00001700
H	-0.02497900	2.30946000	-0.00000300
55 H	-0.75923500	-1.91901600	0.00000900
H	1.70800500	-2.34855000	0.00002100
H	3.28822500	-0.43337200	-0.00004300
C	-1.99222000	0.46858200	0.00000200
O	-2.84809500	-0.39574200	-0.00002300
60 H	-2.27356200	1.54615500	0.00002000

Table S3. Cartesien coordiantes of metal free phosphonate

P	-0.99269600	-0.09891500	-0.45059100
65 O	-1.73723400	0.06895600	0.86320100
O	0.32011400	-1.26708100	-0.13802200
O	0.24123800	1.16751600	-0.52825900
C	1.54857600	-0.65315900	0.15694300
C	1.26969700	0.84221000	0.37999400
70 H	2.02111500	-1.11091700	1.04534000
H	2.25708200	-0.77610700	-0.68722500

H	2.15763800	1.46364200	0.18129600
H	0.95202200	1.01767300	1.42246700

Table S4. Cartesien coordiantes of lithium phosphonate

5	C	-1.54205500	0.75793600	-0.17168400
	C	-1.46468600	-0.55725400	0.60451100
	H	-2.05411600	1.54887000	0.38977000
	H	-2.06217500	0.61406500	-1.12740400
10	H	-2.39182500	-1.13588800	0.55135500
	H	-1.22432000	-0.38079100	1.66427500
	P	0.87878300	-0.37474000	-0.55684200
	O	1.78521200	0.01837500	0.64791600
	O	-0.18754400	1.14433000	-0.41565200
15	O	-0.42941300	-1.30344800	-0.03326100
	Li	1.08169600	1.63223000	0.89521100

Table S6. Cartesien coordiantes of sodium phosphonate

20	C	-1.29073200	1.23140000	-0.34275000
	C	-1.70150800	0.27086000	0.77280800
	H	-1.26864700	2.27772300	-0.01154700
	H	-1.98455800	1.15226200	-1.19156300
	H	-2.78437900	0.24751000	0.93419400
25	H	-1.21643600	0.54286600	1.72460000
	P	0.18126000	-1.00613000	-0.54570300
	O	1.39087600	-1.00213700	0.41905900
	O	0.01736800	0.82259900	-0.73844400
	O	-1.27774700	-1.01391600	0.33280200
30	Na	1.94950700	1.03687700	0.36746900

Table S7. Cartesien coordiantes of potassium phosphonate

	C	-1.23624200	1.46494900	-0.38119800
35	C	-1.81833300	0.72655800	0.82351800
	H	-0.88526500	2.47484500	-0.12470100
	H	-1.99535400	1.55892700	-1.17247800
	H	-2.84159100	1.03978300	1.05908700
	H	-1.19390500	0.88939300	1.71878100
40	P	-0.49322900	-1.10125000	-0.52151900
	O	0.71351300	-1.43919300	0.37460200
	O	-0.14455400	0.67055700	-0.82700900
	O	-1.82968100	-0.64231200	0.44800500
	K	2.24883000	0.45759700	0.19596800

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Table S8. Cartesien coordiantes of free-TS-2

	C	0.23932700	0.39589100	-0.67704600
	Si	-0.01428800	2.20318500	-0.04645300
50	C	1.34479900	3.26039600	-0.87150600
	H	1.20527300	4.33044100	-0.66603900
	H	2.34314600	2.97844800	-0.51486900
	H	1.32813900	3.11996600	-1.95871500
	C	-1.69192200	2.78888400	-0.69557400
55	H	-1.72571600	2.65911500	-1.78218600
	H	-2.49949900	2.18558400	-0.26908000
	H	-1.87086100	3.84609800	-0.45818000
	C	0.07310500	2.49423100	1.83282700
	H	1.10032700	2.41209700	2.20901600
60	H	-0.28913600	3.50146400	2.08168400
	H	-0.54191500	1.76257600	2.36871600
	P	-1.29625800	-0.75266800	0.79212900
	O	-1.43378400	-0.75924800	2.29598100
	O	-2.80087400	-0.32559200	0.08917200
65	O	-1.36176400	-2.32686400	0.11520300
	C	-3.09898200	-1.18964700	-0.99890800
	C	-2.58302500	-2.56621800	-0.56745500
	H	-4.18404700	-1.18871800	-1.17333100
	H	-2.57775500	-0.84813600	-1.90232400
70	H	-2.39612400	-3.22784000	-1.42356300

H	-3.30642900	-3.05666200	0.10449900
O	-0.21201800	0.23554900	-1.85156200
C	1.50110600	-0.37516700	-0.29424600
C	2.19073200	-1.03069800	-1.32325900
5 C	2.05361700	-0.39526200	0.99726900
C	3.39864300	-1.68426100	-1.07584300
H	1.74134300	-1.00988900	-2.31132800
C	3.26166500	-1.04481000	1.24526700
H	1.50949500	0.06220300	1.81862300
10 C	3.94482600	-1.69080900	0.20901300
H	3.91785100	-2.18977700	-1.88911700
H	3.66650100	-1.05920300	2.25560800
H	4.88748600	-2.19827500	0.40538700

15 **Table S9. Cartesien coordiantes of Li-TS-2**

C	2.46945500	-2.41057900	-0.93844200
C	3.48644400	-1.27789800	-0.76969000
H	2.91293800	-3.39877100	-0.78477800
20 H	1.99902100	-2.37922400	-1.93004100
H	4.00928600	-1.03132600	-1.69731900
H	4.21996200	-1.51210900	0.01155200
P	1.43357400	-0.61666200	0.60517900
O	1.84014600	-0.59446600	2.08845300
25 O	1.47072100	-2.19866800	0.06782400
O	2.70692500	-0.13543500	-0.37351700
Li	0.65696400	0.37684000	3.03242600
C	-0.55458600	0.65573900	0.65853100
Si	-0.15994100	2.15537000	-0.51198500
30 C	0.25320800	1.69351100	-2.30185000
H	0.52042000	2.60115800	-2.85833400
H	1.11118200	1.01424400	-2.34931200
H	-0.59175500	1.22767100	-2.82006200
C	1.29163100	3.09507600	0.24972300
35 H	2.21434800	2.50458800	0.22142400
H	1.47597200	4.02769900	-0.29775600
H	1.07922500	3.35493000	1.29255000
C	-1.71968100	3.23036800	-0.47365400
H	-1.96702800	3.51903300	0.55390500
40 H	-1.57611400	4.14811900	-1.05742300
H	-2.58432400	2.70116800	-0.89039300
O	-0.57075200	1.00858900	1.90841300
C	-1.58390500	-0.37516700	0.23503800
C	-2.66384700	-0.62494500	1.09406500
45 C	-1.55091800	-1.02739400	-1.00810600
C	-3.68239500	-1.50363400	0.72250300
H	-2.69454300	-0.10924100	2.04794200
C	-2.56713100	-1.90444300	-1.37892500
H	-0.71181800	-0.86752700	-1.67834100
50 C	-3.63906800	-2.14630000	-0.51486300
H	-4.51355000	-1.68264000	1.40020500
H	-2.51906000	-2.40815000	-2.34099400
H	-4.43104800	-2.83155500	-0.80536000

55 **Table S10. Cartesien coordiantes of Na-TS-2**

C	1.79832500	-2.81654300	-0.97786900
C	2.96307100	-1.84241700	-1.18001600
H	2.13655800	-3.83895900	-0.78366600
60 H	1.12823300	-2.82141700	-1.84813200
H	3.29953600	-1.78859400	-2.21881000
H	3.81291500	-2.09812000	-0.53485300
P	1.35371100	-0.71861400	0.46395000
O	2.05096500	-0.58020300	1.81673500
65 O	1.08564000	-2.34575300	0.16995400
O	2.44152100	-0.55620500	-0.80629200
C	-0.43255500	0.73373800	0.47205000
Si	0.00613200	2.05034000	-0.89006200
C	0.16753800	1.41056400	-2.66812700
70 H	0.47033500	2.23543600	-3.32634100
H	0.93101700	0.62925200	-2.74428300

	H	-0.77861600	1.01437000	-3.05260000
	C	1.63174200	2.87230500	-0.37788800
	H	2.47070000	2.16950100	-0.43425600
	H	1.86065500	3.71983500	-1.03569900
5	H	1.56450600	3.25326000	0.64734100
	C	-1.40496700	3.31318900	-0.81338400
	H	-1.52161200	3.69958600	0.20483400
	H	-1.21162400	4.16219300	-1.48094900
	H	-2.35965700	2.86445600	-1.11188400
10	Na	1.03883100	0.77904600	3.12558900
	O	-0.38518500	1.28273500	1.64947800
	C	-1.58727800	-0.22517600	0.21659400
	C	-2.62444200	-0.28051400	1.15740700
	C	-1.70291600	-0.99668100	-0.95091000
15	C	-3.74201400	-1.08890600	0.94383500
	H	-2.53859000	0.33153500	2.04908400
	C	-2.81866900	-1.80217100	-1.16666800
	H	-0.90734600	-0.97932700	-1.69060300
	C	-3.84465200	-1.85344900	-0.21858100
20	H	-4.53754200	-1.11640400	1.68495900
	H	-2.88605600	-2.39722700	-2.07414900
	H	-4.71471100	-2.48266200	-0.38753400

Table S11. Cartesien coordiantes of K-TS-2

25	C	-1.19109800	3.23315800	0.31984400
	C	-0.22376700	3.34702100	1.50106400
	H	-1.43321400	4.20732300	-0.11703100
	H	-2.12185100	2.73119200	0.61552100
30	H	-0.73220600	3.52683700	2.45277500
	H	0.51818300	4.13833100	1.33227400
	P	0.61209400	1.40696600	0.03090200
	O	1.97439700	1.70669900	-0.58468100
	O	-0.51337400	2.44718000	-0.66193600
35	O	0.43423900	2.07245800	1.57082800
	C	0.11608800	-0.85215300	-0.32352800
	Si	0.85603200	-1.71090900	1.24924500
	C	0.23951400	-1.12441100	2.94391900
	H	0.83452100	-1.59661800	3.73669200
40	H	0.32959500	-0.03875500	3.05456700
	H	-0.80737800	-1.40128900	3.11256700
	C	2.73544100	-1.44461700	1.15574600
	H	2.98178800	-0.38054800	1.05790800
	H	3.23196300	-1.82060100	2.05841200
45	H	3.15712400	-1.98695100	0.29985000
	C	0.48564200	-3.56074100	1.05804900
	H	0.82167500	-3.92319300	0.08015600
	H	0.99287400	-4.14901700	1.83302700
	H	-0.58916100	-3.76144100	1.13716600
50	K	2.83732300	0.00124900	-2.20730500
	O	0.81301400	-1.15348000	-1.36794400
	C	-1.39123700	-0.75776800	-0.49453400
	C	-1.95154800	-1.16367100	-1.71245200
	C	-2.25298900	-0.34927600	0.53656900
55	C	-3.33427900	-1.15845300	-1.89949400
	H	-1.27869500	-1.48495800	-2.50071800
	C	-3.63449900	-0.34494500	0.35144900
	H	-1.83728400	-0.01071600	1.48155700
	C	-4.18253500	-0.75041300	-0.86918200
60	H	-3.75158300	-1.47835600	-2.85170400
	H	-4.28587500	-0.02298700	1.16061200
	H	-5.26006400	-0.74900100	-1.01264400

Table S12. Cartesien coordiantes of free-2

65	C	-0.04088600	0.16202900	-0.39836600
	Si	-0.03332500	2.07497200	-0.06062900
	C	1.21235100	2.80426000	-1.29674100
	H	1.11657100	3.89553700	-1.37454800
70	H	2.24638100	2.57224000	-1.01544300
	H	1.02190200	2.36302400	-2.28013400

C	-1.75104000	2.77482000	-0.46143800
H	-2.06617200	2.37814800	-1.43093200
H	-2.49736500	2.47339700	0.28109000
H	-1.73397700	3.87218100	-0.51223000
5 C	0.44504500	2.66307000	1.69483700
H	1.47887300	2.38909600	1.93732100
H	0.35593800	3.75473200	1.78951600
H	-0.20460300	2.19851600	2.44560800
P	-1.22589100	-0.73272300	0.75706100
10 O	-1.07575300	-0.64900700	2.24260800
O	-2.74112500	-0.27386000	0.25869000
O	-1.35253500	-2.27846600	0.14630600
C	-3.12618000	-1.05938300	-0.87514100
C	-2.55167300	-2.46201000	-0.60382700
15 H	-4.22147000	-1.06594300	-0.93699500
H	-2.66812200	-0.62224600	-1.76559300
H	-2.31358300	-2.98950600	-1.53439800
H	-3.24944300	-3.07384100	-0.01297200
O	-0.50158000	0.06227800	-1.66147200
20 C	1.36224200	-0.43858600	-0.16494600
C	2.04846800	-0.88470800	-1.30269700
C	2.00508600	-0.52995100	1.08266300
C	3.34312600	-1.39677200	-1.20496100
H	1.51112600	-0.81100400	-2.24351200
25 C	3.29860300	-1.04416900	1.17928200
H	1.47395600	-0.22481500	1.98004400
C	3.97924500	-1.47682300	0.03604000
H	3.86001900	-1.73821300	-2.10163800
H	3.77685000	-1.11350200	2.15536900
30 H	4.98964700	-1.87479400	0.11505200

Table S13. Cartesien coordiantes of Li-2

C	-0.37335800	-3.22771200	-0.33217800
35 C	0.82593100	-3.03783800	-1.27016700
H	-0.50058100	-4.26713200	-0.01958500
H	-1.30181000	-2.85830300	-0.77964100
H	0.56527200	-3.14294000	-2.32543100
H	1.64662800	-3.72066400	-1.02398500
40 P	0.97312200	-1.22426700	0.49881800
O	2.16795900	-1.29535100	1.43011100
O	-0.07485500	-2.44332100	0.83564000
O	1.26315200	-1.67769600	-1.05437100
Li	1.90828700	0.12189600	2.59629700
45 C	0.22654200	0.49871400	0.60774800
Si	1.13843400	1.80231100	-0.53652900
C	1.07800200	1.48155600	-2.40709300
H	1.66928500	2.24414000	-2.93066900
H	1.49216300	0.50099700	-2.66479300
50 H	0.05630700	1.53462900	-2.79856700
C	2.96224000	1.85882000	-0.01168600
H	3.45325600	0.88182500	-0.09154800
H	3.51779700	2.56027700	-0.64650500
H	3.05810000	2.21040400	1.02256400
55 C	0.31117900	3.45667500	-0.15441400
H	0.27846000	3.62084300	0.92689400
H	0.86406800	4.28412800	-0.61615200
H	-0.71678200	3.48636300	-0.53225700
O	0.51547300	0.93035200	1.88830700
60 C	-1.27057600	0.41044200	0.29422300
C	-2.18458400	0.79940800	1.28081500
C	-1.76586200	-0.01603300	-0.94995000
C	-3.55769300	0.75886700	1.03414500
H	-1.78814200	1.13288400	2.23313500
65 C	-3.13943300	-0.05865000	-1.19418900
H	-1.07574100	-0.31250900	-1.73572300
C	-4.04297500	0.32919600	-0.20207500
H	-4.25255700	1.06575800	1.81247400
H	-3.50332800	-0.38844400	-2.16459000
70 H	-5.11245500	0.30115100	-0.39396100

Table S14. Cartesien coordiantes of Na-2

C	-1.28583100	-3.01909800	-0.15784100
C	-0.43135700	-3.05730200	-1.43186200
H	-1.54793500	-4.01810300	0.20060600
5 H	-2.19450600	-2.42545900	-0.30098100
H	-1.02980300	-3.05266700	-2.34583600
H	0.24446200	-3.92027300	-1.44073100
P	0.66470800	-1.40298300	0.15425800
O	2.04544400	-1.77252900	0.64321400
10 O	-0.46465300	-2.38742500	0.83801200
O	0.34969800	-1.84495100	-1.40329100
C	0.29623000	0.41580800	0.44393600
Si	1.25135600	1.59160700	-0.78994200
C	0.94325900	1.33523900	-2.64851900
15 H	1.59380800	1.99824600	-3.23383900
H	1.14575700	0.30419600	-2.95862800
H	-0.09214600	1.57015300	-2.91889500
C	3.12007700	1.36143600	-0.49074700
H	3.42219200	0.30995800	-0.57333100
20 H	3.69846600	1.92673800	-1.23177900
H	3.40914000	1.74598300	0.49658000
C	0.76054600	3.34972800	-0.30222600
H	0.82342800	3.46263100	0.78459700
H	1.42354400	4.08842400	-0.76943500
25 H	-0.26674400	3.57786400	-0.60686100
Na	2.63705200	-0.28158600	2.14284500
O	0.83701500	0.72194000	1.67038700
C	-1.22376600	0.62681700	0.35717900
C	-1.88479400	1.10622800	1.49510700
30 C	-1.97617700	0.39977100	-0.80858000
C	-3.25884900	1.34810800	1.47345900
H	-1.28650800	1.28370700	2.38174300
C	-3.35139000	0.64111100	-0.82848500
H	-1.48720500	0.03202400	-1.70631700
35 C	-4.00033800	1.11660800	0.31340400
H	-3.75368900	1.72131800	2.36742900
H	-3.91505100	0.46268000	-1.74155100
H	-5.07008000	1.30928000	0.29569300

40 **Table S15. Cartesien coordiantes of K-2**

C	1.30324100	-3.06653700	0.09589700
C	0.74797900	-3.03014600	1.52586800
H	1.43186300	-4.08690900	-0.27614300
45 H	2.25120300	-2.52357600	0.02021900
H	1.53267200	-3.04562800	2.28627600
H	0.04751300	-3.85407900	1.70764100
P	-0.58927900	-1.35053700	0.16432100
O	-2.05495400	-1.65735300	0.00486700
50 O	0.31837300	-2.41211600	-0.71809100
O	0.04516100	-1.77752900	1.63157700
C	-0.18067400	0.42565600	-0.27805000
Si	-0.82249400	1.70560500	1.04730700
C	-0.18752300	1.50305200	2.82863200
55 H	-0.66989800	2.23448500	3.49034200
H	-0.39836000	0.50203800	3.22173200
H	0.89390800	1.66620000	2.89112700
C	-2.72339900	1.59252000	1.11387500
H	-3.06112900	0.56087800	1.26779100
60 H	-3.11488700	2.19798400	1.94065300
H	-3.16769400	1.98445400	0.19004500
C	-0.33723600	3.40883400	0.38436000
H	-0.56683600	3.46175000	-0.68476100
H	-0.88607700	4.20711000	0.89953100
65 H	0.73400000	3.60119200	0.50900200
K	-3.13134100	-0.22688100	-1.82795000
O	-0.92478900	0.70068800	-1.39390200
C	1.33946100	0.55027900	-0.47781800
C	1.79764200	0.96322200	-1.73535900
70 C	2.28692500	0.31431400	0.53378200
C	3.16074100	1.13325000	-1.98015100
H	1.04997300	1.14713300	-2.49906000

	C	3.65102600	0.48319500	0.28771600
	H	1.95860300	-0.00544000	1.51856300
	C	4.09573500	0.89378900	-0.97137100
	H	3.49555700	1.45634500	-2.96370200
5	H	4.36762600	0.29829900	1.08509600
	H	5.15769600	1.03001000	-1.16031500

Table S16. Cartesien coordiantes of free-TS-3

10	C	-0.00850000	0.18000600	-0.17001500
	Si	-0.27513700	2.04569200	-0.02555500
	C	0.95835600	2.95921200	-1.14979400
	H	1.07350500	4.00643600	-0.83650000
	H	1.94722600	2.48785700	-1.10352100
15	H	0.62924800	2.93495800	-2.19286700
	C	-2.05893000	2.63626800	-0.31237700
	H	-2.29690900	2.64316100	-1.38059200
	H	-2.76723800	1.96573500	0.18413100
	H	-2.20675500	3.64818600	0.09075500
20	C	0.14089500	2.71946000	1.74431400
	H	1.17110600	2.46700900	2.03075500
	H	0.03865700	3.81315500	1.81246400
	H	-0.52038800	2.27592600	2.50098700
	P	-1.10766800	-0.98062300	0.73710800
25	O	-0.89863800	-1.22168700	2.19350500
	O	-2.66175400	-0.52794500	0.38296400
	O	-1.15593200	-2.35707200	-0.20487800
	C	-3.04673600	-1.09251600	-0.87724600
	C	-2.39603300	-2.48441500	-0.89759200
30	H	-4.14112100	-1.13975000	-0.91456800
	H	-2.64061700	-0.46607600	-1.67608200
	H	-2.20023300	-2.83044000	-1.91878000
	H	-3.02260100	-3.22670200	-0.38135800
	O	-0.50487700	0.43078700	-1.45387300
35	C	1.41887800	-0.33470600	-0.09866000
	C	2.09941800	-0.55164500	-1.30687600
	C	2.10637600	-0.56715500	1.10761300
	C	3.42450500	-0.98877100	-1.31387600
	H	1.54243900	-0.36335200	-2.21950600
40	C	3.43122100	-1.00088200	1.09645000
	H	1.58563700	-0.42594400	2.05039900
	C	4.10196400	-1.21363600	-0.11311100
	H	3.93331200	-1.15517200	-2.26297400
	H	3.94502400	-1.17674200	2.04042100
45	H	5.13777600	-1.54857800	-0.11672700

Table S17. Cartesien coordiantes of Li-TS-3

	C	2.31505900	-2.61633900	-0.14350700
50	C	1.41836400	-3.11944600	0.99603000
	H	2.85964400	-3.42434100	-0.63868400
	H	3.01930800	-1.85180200	0.20117700
	H	1.92188400	-3.13165000	1.96484700
	H	1.00894000	-4.11319900	0.78249100
55	P	0.00361300	-1.55331300	-0.40664500
	O	-1.17082100	-2.18846000	-1.13293800
	O	1.41860500	-2.02380500	-1.09839300
	O	0.33750400	-2.16728200	1.07233200
	Li	-2.17343700	-0.86255600	-1.89946400
60	C	-0.26403800	0.19716700	-0.25108900
	Si	-2.13523500	0.82096700	0.34125700
	C	-2.25995500	0.06681500	2.09800000
	H	-3.19728200	0.36188500	2.59142800
	H	-2.22653000	-1.02952000	2.07708500
65	H	-1.42428800	0.40347200	2.72299400
	C	-3.82522900	0.21534200	-0.40476200
	H	-3.90304400	-0.88503100	-0.45761000
	H	-4.65953500	0.51868100	0.23904600
	H	-4.03039800	0.63845400	-1.40157700
70	C	-2.12931500	2.69774600	0.54277100
	H	-2.39004900	3.20078400	-0.39481600

H	-2.84634100	3.00586000	1.31345500
H	-1.13969500	3.05727900	0.84551600
O	-1.26592200	0.61279000	-1.24852900
C	0.93770300	1.06249800	-0.13931500
5 C	1.17149200	2.10187400	-1.05625600
C	1.86255300	0.88029600	0.90858100
C	2.30003900	2.91350900	-0.94041900
H	0.45478000	2.26373800	-1.85423600
C	2.99188200	1.69006100	1.01451400
10 H	1.67540500	0.11335400	1.65594900
C	3.22080800	2.71190800	0.08934600
H	2.46044300	3.71019200	-1.66324900
H	3.68805600	1.53273000	1.83524300
H	4.09701700	3.34840000	0.17827800

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Table S18. Cartesien coordiantes of Na-TS-3

C	-2.10620400	2.76416100	-0.10830800
C	-1.31143000	3.09785700	1.16213700
20 H	-2.53278500	3.65252400	-0.58189300
H	-2.89783800	2.03426700	0.09105700
H	-1.92226800	3.07301000	2.06720100
H	-0.81203000	4.07048800	1.08453900
P	0.14122600	1.54365400	-0.21612700
25 O	1.42289900	2.13996300	-0.74811900
O	-1.15342700	2.18230500	-1.01247400
O	-0.31762000	2.05997600	1.27028300
C	0.19060300	-0.24647700	-0.17469200
Si	1.78845400	-1.15966200	0.58391100
30 C	1.79076900	-0.64015900	2.43905300
H	2.59404800	-1.13791400	3.00141900
H	1.92195300	0.44279500	2.56357700
H	0.83699500	-0.90272900	2.91437300
C	3.63263900	-0.73737900	0.14947900
35 H	3.84211500	0.34301300	0.21379200
H	4.30541900	-1.20393500	0.87917100
H	3.94061800	-1.11477300	-0.84001100
C	1.52681600	-3.03390800	0.59505600
H	1.81406800	-3.48762500	-0.35984500
40 H	2.11391100	-3.50218700	1.39469900
H	0.47332800	-3.27867100	0.77115900
Na	2.58140800	0.71036300	-1.90110700
O	1.17110500	-0.76581600	-1.12741600
C	-1.14343800	-0.91958800	-0.19427000
45 C	-1.47461500	-1.81429400	-1.22569000
C	-2.08755000	-0.70717500	0.82935400
C	-2.71394600	-2.45390000	-1.24545700
H	-0.73935600	-2.00448900	-2.00017700
C	-3.32667800	-1.34643100	0.80300400
50 H	-1.83414500	-0.05477000	1.66057600
C	-3.65068900	-2.22184800	-0.23645800
H	-2.94808100	-3.14106400	-2.05550100
H	-4.03618400	-1.17198900	1.60883200
H	-4.61331500	-2.72606500	-0.25107700

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Table S19. Cartesien coordiantes of K-TS-3

C	-1.91359400	2.95265600	-0.10181300
C	-1.26838600	3.14055200	1.27833900
60 H	-2.17725600	3.90349700	-0.57371700
H	-2.79854700	2.30963900	-0.04744300
H	-1.99683800	3.15257400	2.09233500
H	-0.66043900	4.05216800	1.32020800
P	0.19343900	1.49634200	0.01808600
65 O	1.58396600	1.97885200	-0.30009600
O	-0.91578800	2.30613600	-0.90538200
O	-0.42000700	1.99219600	1.45871400
C	0.03797600	-0.28708200	-0.04754400
Si	1.38039600	-1.41681400	0.87991600
70 C	1.06377300	-1.05922600	2.74963500
H	1.68994600	-1.68593400	3.40141500

H	1.26674900	-0.01004000	3.00208700
H	0.01483800	-1.25393300	3.00806800
C	3.28608400	-1.10804400	0.82114000
H	3.51954200	-0.03619500	0.90290200
5 H	3.77736000	-1.59250600	1.67357800
H	3.75490200	-1.51613100	-0.08844600
C	0.99119700	-3.26176200	0.67955000
H	1.44898000	-3.67053600	-0.22867700
H	1.35451100	-3.83526200	1.54142200
10 H	-0.08947900	-3.42840500	0.60366300
K	2.94470300	0.52002500	-1.85722100
O	1.07911700	-0.88181600	-0.87580000
C	-1.34653900	-0.79637800	-0.28229000
C	-1.62496100	-1.60969200	-1.39429900
15 C	-2.39989000	-0.51359100	0.61005800
C	-2.91199900	-2.09672500	-1.62110300
H	-0.81008200	-1.85920000	-2.06557200
C	-3.68585600	-0.99988000	0.37714900
H	-2.19791500	0.07118900	1.50324600
20 C	-3.95360400	-1.79119000	-0.74277600
H	-3.10169100	-2.72264300	-2.49055300
H	-4.47996800	-0.77283300	1.08516400
H	-4.95459800	-2.17643400	-0.91835600

25 **Table S20. Cartesien coordiantes of free-3**

C	0.27669300	-0.29793700	-0.13569100
Si	-0.56155600	2.27662800	0.12686300
C	0.53924700	3.68783400	-0.51026900
30 H	0.26813800	4.64802000	-0.05041200
H	1.59472400	3.49225200	-0.29112800
H	0.44235800	3.80036500	-1.59756200
C	-2.35608700	2.78939300	-0.21449600
H	-2.55743600	2.81650500	-1.29273600
35 H	-3.05108400	2.07478900	0.23932200
H	-2.57815900	3.78533100	0.19209900
C	-0.30306000	2.05699800	1.98245700
H	0.72939100	1.76435300	2.20129400
H	-0.52318300	2.98793000	2.52290200
40 H	-0.95712100	1.26597900	2.36243700
P	-0.90579700	-1.49641000	0.16492400
O	-0.52738600	-2.71530200	0.94850200
O	-2.26423900	-0.71427100	0.79622600
O	-1.73355700	-1.91762100	-1.25156400
45 C	-3.43440500	-0.91546200	0.01599200
C	-3.11245900	-2.05896500	-0.96134900
H	-4.27879600	-1.15637500	0.67503900
H	-3.66788400	0.00755700	-0.53269000
H	-3.68711000	-1.98460000	-1.89254500
50 H	-3.31339300	-3.03741800	-0.49833700
O	-0.22882600	0.89773000	-0.75028800
C	1.70043900	-0.48683100	-0.13642000
C	2.55989500	0.47530100	-0.74286100
C	2.35382000	-1.60219200	0.47368600
55 C	3.94636100	0.34046600	-0.72571900
H	2.11230400	1.31663400	-1.26000200
C	3.73581500	-1.72012100	0.47631000
H	1.74295500	-2.36631800	0.94218100
C	4.56393100	-0.75318600	-0.11518700
60 H	4.55370300	1.10624400	-1.21019100
H	4.18304200	-2.59000600	0.95850700
H	5.64721500	-0.85394900	-0.09984500

Table S21. Cartesien coordiantes of Li-3

65 C	3.82182000	-0.53270100	-0.20074200
C	3.44714900	-1.47169800	0.95948100
H	4.67454200	-0.90034600	-0.77860100
H	4.03502100	0.48277500	0.15275600
70 H	3.94269200	-1.20574800	1.89662400
H	3.66954900	-2.51818200	0.71592700

	P	1.31085300	-1.08577600	-0.34857200
	O	0.90769000	-2.44163800	-0.94514300
	O	2.67078500	-0.48035400	-1.05347700
	O	2.03423300	-1.30363200	1.13003300
5	Li	-0.72935400	-2.22443100	-1.61549700
	C	0.00996000	0.00335600	-0.36869200
	Si	-2.51011900	-0.90760400	0.30105800
	C	-1.89336600	-0.86074700	2.07022300
	H	-2.69246500	-1.14953500	2.76456100
10	H	-1.04439800	-1.53637900	2.21864100
	H	-1.55716000	0.14703000	2.33479600
	C	-3.04610800	-2.66255200	-0.20450200
	H	-2.27197700	-3.41311400	0.01381600
	H	-3.94185400	-2.97893800	0.34333200
15	H	-3.30999300	-2.72219400	-1.27186000
	C	-3.93178700	0.28633700	0.00264100
	H	-4.25089700	0.27432900	-1.04635300
	H	-4.79983100	0.01971500	0.61877200
	H	-3.64111500	1.31204000	0.25152800
20	O	-1.24067900	-0.61197700	-0.80951100
	C	0.04165300	1.43906600	-0.21494800
	C	-0.94112400	2.27368400	-0.80060900
	C	1.05778600	2.08093200	0.53737200
	C	-0.89674500	3.65879900	-0.65395400
25	H	-1.72571600	1.82260900	-1.39975200
	C	1.10527700	3.46527400	0.65791400
	H	1.79504800	1.47620900	1.05845300
	C	0.12778400	4.27344000	0.06850300
	H	-1.66821600	4.26535300	-1.12439400
30	H	1.90309300	3.91864000	1.24274300
	H	0.16058800	5.35379700	0.17793100

Table S22. Cartesien coordiantes of Na-3

35	C	3.72251800	-0.69083600	0.23041200
	C	3.13403500	-1.63856600	1.29192800
	H	4.60337700	-1.10938600	-0.26429800
	H	3.98251200	0.28278900	0.66265600
	H	3.53360200	-1.44840400	2.29161700
40	H	3.30395500	-2.69012200	1.02771800
	P	1.22362700	-1.05812800	-0.25965400
	O	0.84199400	-2.37056000	-0.93360500
	O	2.69355800	-0.49133700	-0.74954200
	O	1.73101400	-1.35827900	1.30074600
45	C	0.03774300	0.15410800	-0.49674800
	Si	-2.36303500	-0.79896300	0.56054500
	C	-1.61791400	-0.40141200	2.23737600
	H	-2.33341600	-0.64542800	3.03304400
	H	-0.69732400	-0.96458200	2.41997400
50	H	-1.37493400	0.66374800	2.31324300
	C	-2.66500600	-2.65580700	0.36191700
	H	-1.71864200	-3.20691900	0.41403600
	H	-3.32835200	-3.04489100	1.14421500
	H	-3.14117200	-2.88657400	-0.60197700
55	C	-3.98167600	0.12985200	0.28038700
	H	-4.36715000	-0.02994000	-0.73438800
	H	-4.75402200	-0.20985100	0.98197600
	H	-3.84969900	1.20789800	0.42162200
	Na	-0.58913300	-1.61678800	-2.38708500
60	O	-1.30338500	-0.37474700	-0.70976000
	C	0.12923700	1.58994500	-0.30160700
	C	-0.98327500	2.42231800	-0.58197700
	C	1.30421500	2.24354700	0.14776700
	C	-0.92081400	3.80583400	-0.42415300
65	H	-1.89849400	1.96960700	-0.94732100
	C	1.35739600	3.62445600	0.29768500
	H	2.18584900	1.65907500	0.38412800
	C	0.24734100	4.42748000	0.01713100
	H	-1.80099900	4.40303800	-0.65492500
70	H	2.28127800	4.08019900	0.64836700
	H	0.29392300	5.50567800	0.14201100

Table S23. Cartesien coordiantes of K-3

C	-3.36009000	1.72408400	0.27372100
C	-2.59739700	2.46194900	1.39027300
5 H	-4.04649700	2.38201800	-0.26801900
H	-3.92248500	0.86936200	0.66923700
H	-3.10570400	2.40384600	2.35651200
H	-2.43311100	3.51611700	1.13148200
P	-0.82557500	1.35661000	-0.03333900
10 O	-0.04841300	2.48635700	-0.68139500
O	-2.36739200	1.23314600	-0.63343500
O	-1.34352300	1.78267900	1.49391200
C	-0.05123300	-0.16104800	-0.17302300
Si	2.45748100	-0.06890700	0.84673700
15 C	2.23193500	1.47568600	1.90101200
H	3.02820500	1.54061500	2.65400400
H	2.26148600	2.38395500	1.28907600
H	1.27114500	1.47106000	2.42637300
C	4.14161200	-0.01954100	-0.01671000
20 H	4.26483400	0.89520100	-0.61178700
H	4.95966900	-0.03975400	0.71375000
H	4.27575000	-0.87971200	-0.68405300
C	2.29828600	-1.61613000	1.90670800
H	2.50921600	-2.52699900	1.33657500
25 H	2.99576300	-1.57292900	2.75317100
H	1.28431000	-1.70926600	2.30945000
K	0.98066700	1.19435200	-2.63454100
O	1.36958400	-0.08765100	-0.45823500
C	-0.64097900	-1.48469400	-0.14905600
30 C	0.05114000	-2.59685600	-0.69441500
C	-1.92347200	-1.74978200	0.39524400
C	-0.51331800	-3.87051400	-0.71654300
H	1.04550800	-2.44678300	-1.10385800
C	-2.48237800	-3.02218700	0.35805500
35 H	-2.47246500	-0.94933200	0.88022000
C	-1.78944200	-4.10156400	-0.19988300
H	0.05610500	-4.69368400	-1.14487400
H	-3.46870400	-3.17752100	0.79123500
H	-2.22683900	-5.09598300	-0.21551800

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Table S24. Cartesien coordiantes of free-TS-4

C	0.61966900	0.36569000	0.29102600
Si	1.76327300	-1.99278300	-1.01072100
45 C	2.98162500	-2.99908700	0.06377500
H	3.37522500	-3.86570300	-0.48625800
H	3.83491800	-2.38533900	0.37758400
H	2.50188600	-3.37668700	0.97625200
C	0.34895900	-3.19185100	-1.41683700
50 H	-0.50592000	-2.99596200	-0.76158700
H	0.00649800	-3.04678700	-2.44427800
H	0.66011700	-4.23703400	-1.28114600
C	2.76341900	-1.50593700	-2.54530000
H	3.68123500	-0.97163200	-2.26864400
55 H	3.06348200	-2.40568400	-3.10139900
H	2.16498500	-0.86809600	-3.19834700
P	-0.45101000	0.03432500	1.66269000
O	-1.40467700	1.10749600	2.06484400
O	-1.18050100	-1.42722900	1.35364500
60 O	0.45177100	-0.56155300	2.94638500
C	-0.71536300	-2.46585100	2.21128400
C	-0.12111200	-1.76527900	3.44084700
H	-1.55938200	-3.11700900	2.46546600
H	0.04775800	-3.05512500	1.68806000
65 H	0.66323000	-2.36014300	3.92160300
H	-0.90221900	-1.53910800	4.18192800
O	1.44327000	-0.73963100	0.05084900
C	1.30940100	1.66053800	0.22735900
C	2.58848300	1.75511900	-0.36984000
70 C	0.71609000	2.87799500	0.65412700
C	3.23307800	2.98042300	-0.52774800
H	3.07421400	0.84632900	-0.70366200

C	1.37143900	4.09471200	0.49498700
H	-0.25613400	2.84738300	1.13403600
C	2.63674300	4.16756600	-0.09876900
H	4.21881400	3.00357800	-0.99120900
5 H	0.88363000	5.00384100	0.84450100
H	3.14092700	5.12351100	-0.22350800
C	-0.58427800	0.47208300	-1.74353500
O	-0.07644500	-0.49378600	-2.35270800
H	-0.13561100	1.47765100	-1.81397500
10 C	-2.03435800	0.48971200	-1.37865200
C	-2.64927300	1.66645400	-0.92770400
C	-2.82516200	-0.65157800	-1.57984300
C	-4.01848700	1.69997100	-0.67141000
H	-2.04096700	2.55356800	-0.77033700
15 C	-4.19365200	-0.61936300	-1.32456500
H	-2.33989200	-1.54969700	-1.94799000
C	-4.79761200	0.55720700	-0.86989400
H	-4.47894700	2.61774300	-0.31191400
H	-4.79619100	-1.51201400	-1.48387200
20 H	-5.86733500	0.58299100	-0.67153900

Table S25. Cartesien coordiantes of Li-TS-4

No coordinates

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Table S26. Cartesien coordiantes of Na-TS-4

C	-1.11702500	2.47713400	2.67986600
C	-2.40153600	1.84049800	2.13568800
30 H	-1.25446100	2.92503900	3.66801700
H	-0.72149100	3.22913200	1.98755000
H	-3.01461500	2.53865300	1.56102200
H	-3.00429000	1.39628900	2.93612800
P	-0.50539000	0.20464400	1.69070700
35 O	-0.51820400	-1.13274900	2.38582400
O	-0.18418500	1.39556500	2.79940900
O	-1.96230100	0.79970700	1.24458800
C	0.50425700	0.21718000	0.23104400
Si	3.05159100	-1.09238400	-0.28695600
40 C	2.93650800	-0.99636500	-2.16108900
H	3.89268700	-1.30108900	-2.60589700
H	2.15927600	-1.66884300	-2.53655500
H	2.71706700	0.01972300	-2.50407300
C	3.24453700	-2.90540100	0.25967300
45 H	2.47699300	-3.55131800	-0.18400900
H	4.21415500	-3.29437300	-0.07442300
H	3.24269000	-3.01384100	1.35551700
C	4.60064300	-0.21060000	0.34683500
H	4.58651100	-0.13098400	1.44039800
50 H	5.49197300	-0.78805500	0.06873200
H	4.72804700	0.79801400	-0.05873100
O	1.70414200	-0.51030900	0.55153600
C	0.67586200	1.51385400	-0.45871700
C	1.93036000	2.14787100	-0.58202800
55 C	-0.43225400	2.17441700	-1.04218800
C	2.07768100	3.35244400	-1.26879400
H	2.79382700	1.70919800	-0.09857300
C	-0.28241800	3.38536400	-1.71357900
H	-1.41367000	1.72233900	-0.96756800
60 C	0.97411700	3.98351800	-1.84362900
H	3.06297600	3.80823000	-1.33780500
H	-1.15744700	3.86004500	-2.15243100
H	1.08849000	4.92251400	-2.37819700
C	-0.45896600	-1.49509000	-1.28234900
65 O	0.11829700	-2.52649300	-0.84860400
H	0.04250900	-0.87199500	-2.03765800
C	-1.93264000	-1.32493300	-1.23891400
C	-2.55114000	-0.41952700	-2.11557500
C	-2.73710000	-2.12071500	-0.40844900
70 C	-3.93846700	-0.28833700	-2.13924200
H	-1.93553100	0.17622700	-2.78495300

C	-4.12199800	-1.98643400	-0.42783100
H	-2.26559700	-2.84503500	0.24806200
C	-4.72793300	-1.06771500	-1.29047000
H	-4.40476800	0.41414800	-2.82535600
5 H	-4.73426500	-2.60307600	0.22529300
H	-5.81024900	-0.96914000	-1.30898200
Na	0.66916700	-2.55698600	1.26161500

Table S27. Cartesien coordiantes of K-TS-4

10	C	-0.79591500	-3.22501400	2.06440100
	C	0.56120800	-3.51047500	1.40970700
	H	-0.96648200	-3.83193500	2.95840600
	H	-1.61914200	-3.37859800	1.35657700
15	H	0.51651600	-4.31632800	0.67268400
	H	1.32936000	-3.74116400	2.15745500
	P	0.25080200	-0.97914700	1.44012900
	O	1.16475300	-0.11923400	2.26662900
	O	-0.74230300	-1.84918500	2.45429300
20	O	0.91769100	-2.29910700	0.72380300
	C	-0.56454100	-0.12938500	0.11627100
	Si	-2.04456400	2.33938000	-0.01285200
	C	-2.33371600	2.27071200	-1.86952500
	H	-2.97001900	3.11341500	-2.17119100
25	H	-1.38122500	2.35092500	-2.40040600
	H	-2.83515600	1.34737000	-2.17535000
	C	-1.21423700	3.98323000	0.45700900
	H	-0.29729100	4.14884200	-0.11846900
	H	-1.89324500	4.81546300	0.23294900
30	H	-0.99844800	4.04963000	1.53379900
	C	-3.70211800	2.34129100	0.90753900
	H	-3.55842300	2.21151400	1.98723500
	H	-4.21080300	3.30240100	0.75555900
	H	-4.38280700	1.55582500	0.56409800
35	O	-1.07239900	1.11257900	0.62617400
	C	-1.54891000	-0.97080800	-0.62610300
	C	-2.92484800	-0.96268000	-0.30936500
	C	-1.13710600	-1.84676600	-1.65065100
	C	-3.83843700	-1.75908200	-0.99703500
40	H	-3.26975400	-0.34491300	0.51197300
	C	-2.04743800	-2.65768000	-2.32861000
	H	-0.08784900	-1.88797600	-1.91895500
	C	-3.40681100	-2.61372400	-2.01506500
	H	-4.89050300	-1.72714800	-0.72254500
45	H	-1.69176900	-3.31709200	-3.11703100
	H	-4.11777600	-3.23591200	-2.55209000
	C	1.11310600	0.92806100	-1.49411800
	O	0.86296500	2.12968900	-1.24609100
	H	0.48350900	0.35768300	-2.18999800
50	C	2.47815200	0.37062600	-1.24157100
	C	2.78682600	-0.98709300	-1.41721000
	C	3.52175700	1.25355500	-0.90557200
	C	4.08414000	-1.45315200	-1.22270900
	H	1.99960500	-1.68542700	-1.67750000
55	C	4.82123900	0.78742100	-0.70761300
	H	3.30913700	2.31935100	-0.86622900
	C	5.10572400	-0.57122000	-0.85779500
	H	4.30058500	-2.51031600	-1.35194100
	H	5.61614000	1.48654200	-0.45869300
60	H	6.11720600	-0.93865200	-0.70674700
	K	1.34559900	2.23723900	1.35810800

Table S28. Cartesien coordiantes of free-4

65	C	0.16487000	0.47521200	-0.01343600
	Si	2.22283800	-0.81954500	-1.38063900
	C	3.97303700	-0.03718100	-0.90374800
	H	4.76875300	-0.46450000	-1.53356700
	H	3.99486800	1.05339500	-1.04085700
70	H	4.26586600	-0.22532200	0.14156900
	C	2.78624600	-2.65361700	-1.13954600

H	2.67755600	-2.94855100	-0.08565400
H	2.16231000	-3.34154100	-1.72109000
H	3.83873900	-2.80610600	-1.41291600
C	2.18566200	-0.27744100	-3.22603500
5 H	1.70852600	0.70821700	-3.32286900
H	3.19328500	-0.18659400	-3.65243600
H	1.60725500	-0.97743200	-3.84052600
P	-0.10297200	-0.03715200	1.77210700
O	-1.49221400	-0.06650300	2.29858900
10 O	0.74276600	-1.42600700	2.03020800
O	0.94128300	0.94142000	2.59931500
C	2.07582000	-1.14759700	2.47871400
C	1.99639100	0.20129900	3.21464500
H	2.38766100	-1.96281200	3.13987100
15 H	2.74268400	-1.09069100	1.61653700
H	2.92510900	0.77219900	3.12078300
H	1.76225400	0.06442700	4.27936100
O	1.53909200	0.40223200	-0.21706600
C	-0.35253200	1.90862600	-0.17361400
20 C	0.49792100	2.88453100	-0.71036100
C	-1.66905500	2.27304300	0.15495000
C	0.04253600	4.18452500	-0.93392300
H	1.51896700	2.60233000	-0.93999000
C	-2.12045700	3.57513400	-0.06774400
25 H	-2.33013100	1.54125100	0.60592200
C	-1.27047100	4.53704900	-0.61688500
H	0.71980300	4.92623900	-1.35324700
H	-3.14295800	3.83770100	0.19615300
H	-1.62568600	5.55117800	-0.78882400
30 C	-0.46916400	-0.50652400	-1.12241000
O	0.49576600	-1.45092100	-1.37543900
H	-0.62675900	0.16765500	-1.98911200
C	-1.80988000	-1.15843100	-0.81566200
C	-3.01447200	-0.57733800	-1.22961900
35 C	-1.85560400	-2.39984700	-0.16726600
C	-4.23806800	-1.20157200	-0.97725700
H	-2.99152300	0.37158600	-1.76056600
C	-3.07464900	-3.02632000	0.08489200
H	-0.91852300	-2.86514600	0.11935400
40 C	-4.27300300	-2.42970600	-0.31587800
H	-5.16281400	-0.73192500	-1.30726300
H	-3.09070300	-3.98798300	0.59398100
H	-5.22401300	-2.92148800	-0.12104500

45 **Table S29. Cartesien coordiantes of Li-4**

C	-0.81346800	2.80833400	2.28125500
C	-1.95082200	1.83616500	2.62903700
H	-0.61419000	3.52526700	3.08077600
50 H	-1.00297200	3.34029400	1.34407100
H	-2.92366700	2.17975900	2.27178800
H	-2.00122900	1.63514900	3.70432000
P	-0.03222500	0.47827000	1.66689300
O	0.65953700	-0.57220200	2.50068500
55 O	0.36261100	1.98917000	2.12271700
O	-1.63607700	0.60306400	1.94462100
Li	1.58614600	-1.89085200	1.60429500
C	0.32292900	0.32301800	-0.16982300
Si	2.94421200	-0.61591300	-0.48906200
60 C	3.16300100	-1.37036000	-2.22140300
H	4.22123900	-1.62092900	-2.37241100
H	2.56626400	-2.27105600	-2.38684700
H	2.90793300	-0.63366400	-2.99419100
C	3.73851700	-1.64628500	0.95604500
65 H	3.42827600	-2.70329600	1.00963300
H	4.82228200	-1.66411800	0.80184400
H	3.60865600	-1.16837800	1.94223100
C	4.28263900	0.77432700	-0.53945900
H	4.33862800	1.33009200	0.40598700
70 H	5.28204600	0.36253900	-0.73742000
H	4.07118000	1.50760800	-1.32852400
O	1.69874300	0.60744700	-0.21299800

C	-0.47160300	1.36948600	-0.94689700
C	0.20643000	2.43610300	-1.55384000
C	-1.86877100	1.29616500	-1.07691100
C	-0.49190600	3.39671700	-2.28749300
5 H	1.28203500	2.49866100	-1.44131800
C	-2.56279100	2.25888500	-1.81115400
H	-2.41788300	0.48901200	-0.60665600
C	-1.87832800	3.31201600	-2.42099000
H	0.05206400	4.21375500	-2.75459200
10 H	-3.64270900	2.18078700	-1.90827700
H	-2.42146400	4.05915400	-2.99386800
C	0.19945200	-1.16078400	-0.71693600
O	1.29565100	-1.82559400	-0.17709500
H	0.34174100	-1.02041600	-1.80370000
15 C	-1.11642600	-1.90875500	-0.54823800
C	-1.92989200	-2.11264700	-1.67207600
C	-1.53685900	-2.45326300	0.67445000
C	-3.12850900	-2.82135500	-1.58111000
H	-1.61452800	-1.71265300	-2.63255800
20 C	-2.73412200	-3.16337100	0.77087400
H	-0.93819900	-2.32091500	1.57032500
C	-3.53628000	-3.35001100	-0.35601900
H	-3.73734800	-2.96713300	-2.46967500
H	-3.03892900	-3.57214400	1.73085500
25 H	-4.46612600	-3.90747100	-0.28051200

Table S30. Cartesian coordinates of Na-4

C	1.72433500	-2.45096800	2.30802700
30 C	2.54598000	-1.18386800	2.59122500
H	1.76212500	-3.16822500	3.13121600
H	2.03359400	-2.93721800	1.37802200
H	3.56494900	-1.24926900	2.20383900
H	2.57245800	-0.94621700	3.66036300
35 P	0.28682100	-0.46077200	1.67047600
O	-0.64512200	0.37444200	2.50511700
O	0.35997800	-2.00912100	2.17211700
O	1.87258400	-0.11423200	1.89603800
C	-0.11015100	-0.49617300	-0.16623500
40 Si	-2.86226400	-0.38058000	-0.64041700
C	-3.14365700	-0.02378400	-2.49265300
H	-4.21289500	-0.12319600	-2.72149700
H	-2.81901400	0.97399200	-2.80342000
H	-2.62510900	-0.76635700	-3.11280300
45 C	-4.13708400	0.53295100	0.51816000
H	-4.14621800	1.63101600	0.42890400
H	-5.14509000	0.19883500	0.24953800
H	-4.02421900	0.24068700	1.57697100
C	-3.72112500	-2.11418800	-0.49844000
50 H	-3.68549900	-2.51212300	0.52519200
H	-4.77905700	-2.06518200	-0.79251800
H	-3.23684800	-2.85837600	-1.14395200
O	-1.33331100	-1.17864200	-0.17520100
C	0.97179800	-1.29104400	-0.89627600
55 C	0.68387100	-2.58211800	-1.35985100
C	2.25471400	-0.76339700	-1.11587700
C	1.65251200	-3.32453300	-2.03824700
H	-0.30482300	-2.98795900	-1.18122400
C	3.21966700	-1.50778500	-1.79545600
60 H	2.50278400	0.22834400	-0.75471900
C	2.92306900	-2.79107300	-2.25957700
H	1.41095200	-4.32272400	-2.39477100
H	4.20504100	-1.08063800	-1.96415200
H	3.67592300	-3.36880500	-2.78969300
65 C	-0.43313900	0.90651000	-0.83506300
O	-1.72350500	1.21870900	-0.41598100
H	-0.43821200	0.64895400	-1.90974100
C	0.52975900	2.07917900	-0.68732400
C	1.09911400	2.62654600	-1.84655900
70 C	0.82750500	2.69618200	0.53875700
C	1.93470500	3.74284200	-1.79061000
H	0.87601300	2.17151400	-2.80835600

C	1.66192800	3.81346000	0.60067500
H	0.43724200	2.29358000	1.46852100
C	2.21863800	4.34379600	-0.56400800
H	2.35838000	4.14494100	-2.70730100
5 H	1.88328400	4.26412200	1.56505600
H	2.86737900	5.21425900	-0.51509400
Na	-2.12939700	1.72830100	1.65450900

Table S31. Cartesien coordiantes of K-4

10 C	2.77870400	-1.02242200	2.48903500
C	2.71537700	0.49048000	2.74880800
H	3.16248700	-1.57990200	3.34679300
H	3.37176300	-1.25629200	1.59971600
15 H	3.61713000	1.01017500	2.41715300
H	2.53047200	0.71348800	3.80582500
P	0.51464200	-0.21645800	1.67315400
O	-0.78734200	-0.03498100	2.39597600
O	1.41905600	-1.43808700	2.26590700
20 O	1.60559600	0.97742400	1.97072400
C	0.37108600	-0.50207500	-0.17647500
Si	-1.86728700	-2.04503600	-0.82401400
C	-2.06813500	-2.00966600	-2.72277100
H	-2.81215200	-2.75938400	-3.02251800
25 H	-2.38965800	-1.03698000	-3.11020000
H	-1.13067500	-2.28659900	-3.22209600
C	-3.59035100	-2.05773700	0.08302700
H	-4.23654000	-1.20105400	-0.15942000
H	-4.13532700	-2.95823800	-0.22108800
30 H	-3.47861300	-2.14389600	1.17647400
C	-1.54028700	-3.94324700	-0.55252400
H	-1.40929300	-4.18854900	0.51090200
H	-2.37328900	-4.55467000	-0.92773600
H	-0.63029700	-4.27700000	-1.06773100
35 O	-0.19894100	-1.77962000	-0.20821400
C	1.76746500	-0.50028300	-0.79857000
C	2.35285300	-1.71656800	-1.17578400
C	2.48519500	0.68857900	-1.00670400
C	3.62296100	-1.74387700	-1.75549600
40 H	1.79456000	-2.63054900	-1.01028800
C	3.75310000	0.65827600	-1.58864600
H	2.05698600	1.64104300	-0.71321400
C	4.32796200	-0.55768400	-1.96469100
H	4.06019700	-2.69606400	-2.04564900
45 H	4.29134200	1.58909900	-1.74966700
H	5.31578300	-0.57887400	-2.41799600
C	-0.66390200	0.40345000	-0.96381400
O	-1.91774700	-0.11438200	-0.65411000
H	-0.40662300	0.17441300	-2.01458600
50 C	-0.63749300	1.92646900	-0.85705200
C	-0.61750900	2.66551700	-2.05007800
C	-0.72040100	2.64474900	0.34888100
C	-0.68039900	4.05935200	-2.04863700
H	-0.55684800	2.13303900	-2.99592100
55 C	-0.78111000	4.04079700	0.35590000
H	-0.70074500	2.12750100	1.30250400
C	-0.76545200	4.75561900	-0.84243100
H	-0.66235200	4.60013200	-2.99140800
H	-0.82733500	4.56929900	1.30536000
60 H	-0.81079600	5.84139000	-0.83530700
K	-3.09688200	0.58235000	1.48341300

Table S32. Cartesien coordiantes of free-TS-5

65 C	0.10051900	0.10391000	1.05375200
Si	-3.15863800	-0.64982500	0.81255500
C	-3.58115000	1.18546500	0.81035300
H	-4.66636600	1.33694600	0.72637200
H	-3.22285000	1.66827300	1.72413900
70 H	-3.08386400	1.68704100	-0.02745900
C	-4.48909200	-1.55573300	-0.19356500

H	-4.48573000	-1.20807400	-1.23377600
H	-4.31301000	-2.63807100	-0.20721200
H	-5.49354400	-1.37861600	0.21377200
C	-3.16276600	-1.35137100	2.57540200
5 H	-2.40198600	-0.85804100	3.18884200
H	-4.13949200	-1.18225200	3.04845600
H	-2.97197900	-2.43205600	2.58837000
P	0.05193200	1.49692300	-1.40873100
O	0.01424900	1.04103900	-2.85531700
10 O	-1.24813500	2.63848500	-1.20047000
O	1.21673400	2.76435400	-1.20543100
C	-0.78771600	3.93649300	-0.88512700
C	0.63185200	4.03033200	-1.45230300
H	-1.46087000	4.68575600	-1.32831500
15 H	-0.77260100	4.08897500	0.20716700
H	1.22949800	4.80974500	-0.95976400
H	0.59873900	4.24603700	-2.53342200
O	-0.70615300	0.76216500	1.72117800
C	1.58015300	0.29314600	1.31284100
20 C	1.92402700	0.85600100	2.55171600
C	2.61209900	-0.07039300	0.43440700
C	3.25826000	1.03695600	2.91423300
H	1.11863100	1.15414400	3.21515000
C	3.94560800	0.11105000	0.79625900
25 H	2.37378700	-0.46618400	-0.54486200
C	4.27678100	0.66038900	2.03782000
H	3.50211100	1.47516100	3.88014100
H	4.73040100	-0.16622100	0.09636500
H	5.31978300	0.80269900	2.31342400
30 C	-0.45643800	-1.26201300	0.52810800
O	-1.75367200	-1.09630900	0.00250900
H	-0.52069300	-1.82349100	1.47965300
C	0.35882800	-2.13412200	-0.41092200
C	1.10564900	-3.19342000	0.12184500
35 C	0.35899200	-1.93948500	-1.80028500
C	1.85674600	-4.03417300	-0.70134200
H	1.10163300	-3.36081500	1.19753400
C	1.11021700	-2.78179500	-2.62185300
H	-0.18746800	-1.10919300	-2.23735800
40 C	1.86038900	-3.82957200	-2.08158500
H	2.43125600	-4.84855100	-0.26450300
H	1.11242300	-2.60628400	-3.69504100
H	2.44222100	-4.48106500	-2.73073900

45 **Table S33. Cartesien coordiantes of Li-TS-5**

C	1.19854800	-3.34929800	1.82340800
C	1.90786700	-2.35002200	2.74260500
H	0.91945900	-4.27087900	2.34267200
50 H	1.81772400	-3.59935900	0.95274200
H	2.99154600	-2.49186700	2.76844300
H	1.51028700	-2.39379300	3.76430600
P	0.13113500	-1.03807100	1.44725000
O	-0.93894100	-0.52707000	2.44180500
55 O	0.00008200	-2.69754000	1.38360900
O	1.63593100	-1.05650400	2.17509400
Li	-2.08839900	0.68848100	1.79494100
C	-0.12713900	-0.31012900	-0.83742300
Si	-3.06830500	-0.10627000	-0.71942800
60 C	-3.40887400	0.19121100	-2.55104200
H	-4.48439400	0.10921700	-2.75008500
H	-3.10381400	1.20309700	-2.84591600
H	-2.88043900	-0.52302700	-3.18792400
C	-4.49197200	0.82760800	0.21030900
65 H	-4.54351300	1.88932300	-0.05939500
H	-5.46400600	0.37152000	-0.01775000
H	-4.41293400	0.78126400	1.31369300
C	-3.36079400	-1.86941200	-0.07713300
H	-2.79436500	-2.06728600	0.84129400
70 H	-4.42315000	-2.02707600	0.14614800
H	-3.03188000	-2.61256900	-0.80856300
O	-1.11727200	-1.00005400	-1.25002300

C	1.23223800	-0.62065700	-1.40528600
C	1.29359900	-1.52511400	-2.47590100
C	2.42072500	-0.03640200	-0.93929200
C	2.51365100	-1.82888700	-3.07882500
5 H	0.37138500	-1.97926300	-2.82071900
C	3.63799000	-0.33987500	-1.54627700
H	2.40222600	0.63418600	-0.08830400
C	3.68941000	-1.23402400	-2.61872300
H	2.54498300	-2.52979100	-3.90904800
10 H	4.55055300	0.11857400	-1.17458900
H	4.64137600	-1.46859000	-3.08807500
C	-0.59938000	1.15771700	-0.63216800
O	-1.89541000	1.04703800	-0.03316000
H	-0.74520500	1.48886700	-1.67218400
15 C	0.25200300	2.22667800	0.02452700
C	0.82786300	3.19900200	-0.80783900
C	0.48553700	2.32227400	1.40607300
C	1.61892500	4.22316800	-0.28870500
H	0.65294300	3.15148200	-1.87990500
20 C	1.27118900	3.35142400	1.92932100
H	0.08979900	1.57995300	2.09072200
C	1.84231200	4.30477100	1.08618800
H	2.05307800	4.96037800	-0.95873500
H	1.44174200	3.39811000	3.00152600
25 H	2.45374300	5.10379100	1.49655800

Table S34. Cartesien coordiantes of Na-TS-5

C	2.02423800	-2.95300300	1.86340800
30 C	2.49363400	-1.80398100	2.76041200
H	1.99352600	-3.91104400	2.39202300
H	2.66651600	-3.05212000	0.97844900
H	3.58158600	-1.69123100	2.76992200
H	2.13362400	-1.93098800	3.78983700
35 P	0.42868500	-0.96121200	1.48640400
O	-0.70591000	-0.69095800	2.49404300
O	0.69519400	-2.61532500	1.45620600
O	1.91917700	-0.61991400	2.18800700
C	0.08043300	-0.38398000	-0.91422600
40 Si	-2.85912500	-0.81162200	-0.95080100
C	-3.08318600	-0.83203300	-2.82534400
H	-4.08844300	-1.18783000	-3.08245600
H	-2.98682000	0.18071500	-3.23728200
H	-2.34735200	-1.47063700	-3.32025300
45 C	-4.55994900	-0.14138700	-0.29709300
H	-4.79192100	0.85775800	-0.68614800
H	-5.37267100	-0.81532400	-0.59852000
H	-4.64099400	-0.08286700	0.80529800
C	-2.79257300	-2.49102500	-0.06964900
50 H	-2.26158600	-2.42539800	0.88879000
H	-3.80352100	-2.86812600	0.13001200
H	-2.24723600	-3.22670800	-0.66678800
O	-0.68913000	-1.31063100	-1.30918400
C	1.51109200	-0.39940200	-1.37876700
55 C	1.86341600	-1.35065600	-2.34841700
C	2.48902600	0.49722400	-0.91993800
C	3.15968500	-1.39659200	-2.85970600
H	1.10331600	-2.04526800	-2.68827000
C	3.78265400	0.45143600	-1.43601500
60 H	2.25129900	1.21176600	-0.14102000
C	4.12264300	-0.49231800	-2.40862200
H	3.41672600	-2.13761400	-3.61235100
H	4.53018800	1.15026400	-1.06996400
H	5.13351100	-0.52527100	-2.80702900
65 C	-0.72208900	0.94553200	-0.82659800
O	-2.01370000	0.59574500	-0.32897600
H	-0.83232600	1.19368800	-1.89532500
C	-0.20419900	2.21019300	-0.16523900
C	0.07270600	3.31148300	-0.98921700
70 C	-0.02301800	2.36536200	1.21977100
C	0.52204200	4.52156500	-0.46010300
H	-0.06695400	3.21889400	-2.06354600

C	0.42187100	3.57729200	1.75266500
H	-0.17950800	1.53079000	1.89517100
C	0.69593900	4.66072500	0.91709200
H	0.73039800	5.35542900	-1.12514400
5 H	0.56737100	3.66513000	2.82627100
H	1.04391700	5.60160900	1.33468700
Na	-2.42785400	0.41230300	1.86468600

Table S35. Cartesien coordiantes of K-TS-5

10 C	2.33377800	-2.72440300	1.99589200
C	2.64746000	-1.53008400	2.90146300
H	2.37193000	-3.67763400	2.53375100
H	3.02841800	-2.76785000	1.14578100
15 H	3.71926300	-1.32008200	2.96902300
H	2.24661800	-1.68477100	3.91268500
P	0.57737300	-0.89067800	1.51295900
O	-0.62512300	-0.72207200	2.45656200
O	1.00203300	-2.51917700	1.52242000
20 O	2.00028700	-0.40981600	2.28627100
C	0.32571700	-0.40816700	-0.96840400
Si	-2.56953600	-1.15243000	-1.29271300
C	-2.47524200	-1.29492800	-3.17502100
H	-3.39001100	-1.75776800	-3.56561100
25 H	-2.39930600	-0.30112500	-3.63520800
H	-1.61507500	-1.88400000	-3.50135700
C	-4.41939800	-0.66457200	-0.99806500
H	-4.67006100	0.29546200	-1.46673400
H	-5.07809800	-1.42700200	-1.43544800
30 H	-4.72431200	-0.59622700	0.06051000
C	-2.42374400	-2.75874700	-0.29372200
H	-1.94509300	-2.58799000	0.67901600
H	-3.40666000	-3.21576400	-0.12111100
H	-1.78521100	-3.47859400	-0.81371500
35 O	-0.26716500	-1.44635400	-1.36869100
C	1.78446400	-0.24234000	-1.29965700
C	2.35824500	-1.19186000	-2.15925800
C	2.58235800	0.81033900	-0.82476200
C	3.69388700	-1.08699000	-2.54481300
40 H	1.73647400	-2.00667900	-2.51331800
C	3.91569400	0.91573100	-1.21572700
H	2.17450600	1.53226300	-0.12773700
C	4.47668100	-0.02977800	-2.07788600
H	4.12249100	-1.83024300	-3.21247600
45 H	4.52145300	1.73452300	-0.83630400
H	5.51801200	0.05509000	-2.37820600
C	-0.64961500	0.80683600	-0.99841700
O	-1.93590800	0.32009500	-0.61977700
H	-0.67416000	1.01959600	-2.08105600
50 C	-0.36470800	2.14274100	-0.33253700
C	-0.19997400	3.26386500	-1.15962000
C	-0.29682500	2.33804500	1.05800600
C	0.03191400	4.53355100	-0.62922200
H	-0.25260300	3.13910800	-2.23859300
55 C	-0.06717300	3.60843200	1.59133500
H	-0.37318500	1.49409800	1.73531300
C	0.09643900	4.71214900	0.75257000
H	0.15945500	5.38111300	-1.29744600
H	-0.00030500	3.72876800	2.66992600
60 H	0.27801700	5.69823600	1.17163500
K	-2.82854600	0.26164900	1.88437200