Supporting Information

Theoretical Investigation of Promising Molecules of Obtaining Complexes with Planar Tetracoordinate Carbon

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Table S1 The multiplicity, energies including zero point energy (E, in Hartree), relative energies (E_r, in kcal/mol).

Isomers	Multiplicity	E	E_r
A1	1	-180.10836	16.4
	3	-179.99772	85.8
A2	1	-180.10592	17.9
	3	-180.02309	69.9
A3	1	-180.05187	51.8
	3	-180.00846	79.0
A4	1	-180.10366	19.3
	3	-180.07127	39.6
A5	5	-179.93728	123.7
A6	3	-179.99661	86.5
A7	1	-180.09314	25.9
	3	-180.06281	44.9
A8	1	-180.05156	52.0
	3	-180.05373	50.6
A9	1	-180.13443	0.0
	3	-180.07819	35.3
A10	1	-180.13357	0.5
	3	-180.06548	43.3

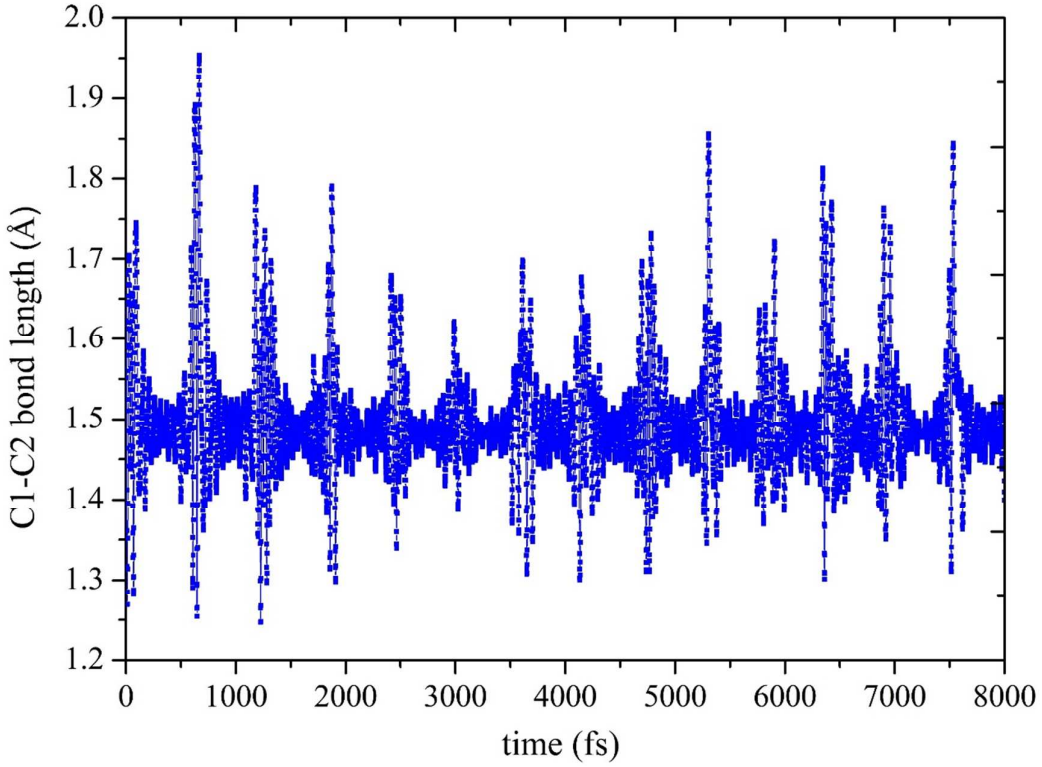

Figure S1. The evolution of C1-C2 bond length within 8000 fs from ab initio Molecular Dynamics (AIMD) simulations at T= 1273 K.

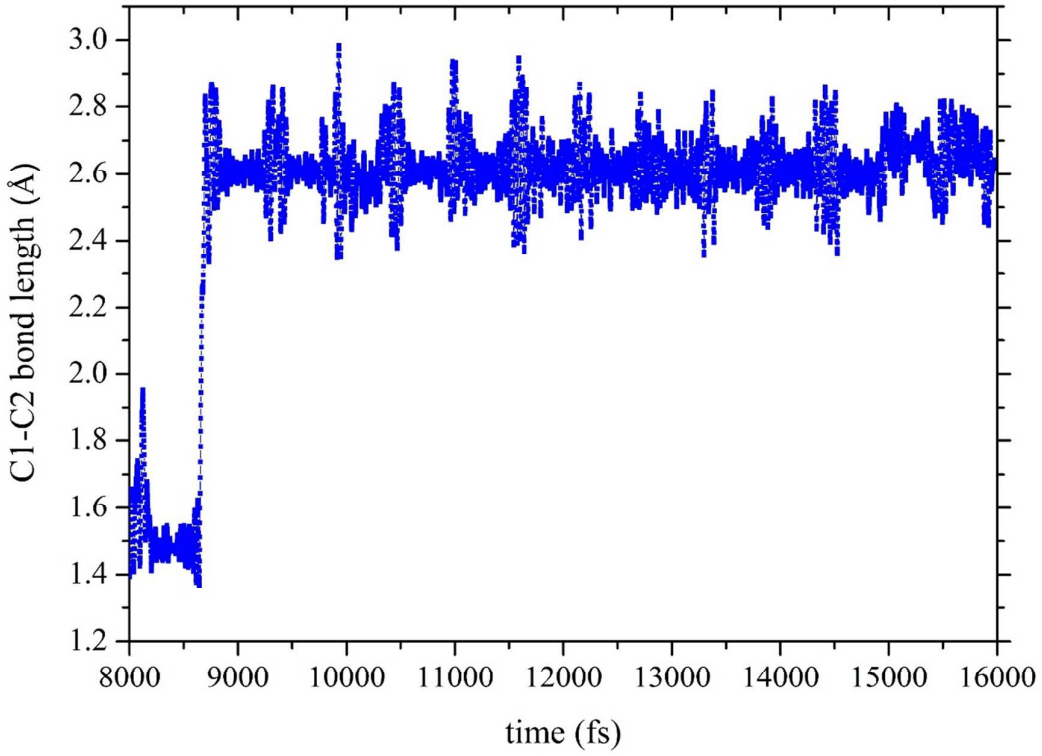

Figure S2. The evolution of C1-C2 bond length from 8000 fs to 16000 fs by ab initio Molecular Dynamics (AIMD) simulating at T= 1273 K.

Cartesian coordinates for all the species and energies

A1

E=-180.18475 a.u.

C	-0.004043	-1.910805	0.000000
H	-0.917644	-2.505764	0.000000
H	0.903620	-2.514744	0.000000
C	0.001872	-0.631117	0.735647
C	0.001872	-0.631117	-0.735647
B	0.009068	0.635181	0.000000
C	0.001872	2.188799	0.000000
H	0.494541	2.594180	-0.889397
H	-1.029845	2.561685	0.000000
H	0.494541	2.594180	0.889397

A2

E=-180.18344 a.u.

C	1.862876	-0.026575	-0.000085
H	2.459858	-0.146687	0.903192
H	2.459399	-0.146656	-0.903677
C	0.530596	-0.733217	0.000078
B	0.656425	0.928989	0.000030
C	-0.540358	0.087888	0.000263
C	-2.018651	-0.029058	-0.000112
H	-2.329049	-1.077179	-0.001824
H	-2.439685	0.464211	0.882124
H	-2.439426	0.467134	-0.880834

A3

E=-180.12533 a.u.

C	-1.637531	-0.693597	0.000001
H	-1.816318	-1.253698	0.918891
H	-1.816174	-1.253617	-0.918975
C	-0.480234	0.364770	0.000039
C	-1.792418	0.789650	-0.000032
B	0.886976	0.170962	0.000061
C	2.388071	-0.100580	-0.000003
H	2.687012	-0.673413	-0.886238
H	2.956012	0.838005	-0.000042
H	2.687269	-0.673549	0.886027

A4

E=-180.17738 a.u.

C	2.162943	-0.677515	0.006815
H	2.612937	-1.016221	-0.902956
H	2.617097	-0.910188	0.947298
C	0.861647	0.144844	-0.037386
C	0.178578	1.603185	-0.011226
B	-0.730684	0.187542	0.066564
C	-2.204436	-0.550632	-0.008625
H	-2.774386	-0.298568	0.861157
H	-2.724355	-0.220727	-0.883694
H	-2.070272	-1.611297	-0.052096

A5

E=-180.00863 a.u.

C	2.006197	-0.430884	-0.000001
H	2.429549	-0.887653	0.907175
H	2.429319	-0.887573	-0.907333
C	-2.375698	0.072432	0.000000
H	-2.570900	0.699873	0.885279
H	-2.571050	0.699365	-0.885626
H	-3.116890	-0.737377	0.000281
C	-1.004753	-0.439006	-0.000007
C	1.580856	0.962757	-0.000017
B	0.432071	0.024315	0.000075

A6

E=-180.06912 a.u.

C	-1.564556	-0.730883	0.000119
H	-1.660780	-1.322940	-0.911829
H	-1.660083	-1.321651	0.912956
C	2.084560	-0.237808	-0.000343
H	2.695002	-0.008166	0.881225
H	1.866992	-1.318299	-0.000799
H	2.693995	-0.007370	-0.882389
C	0.848082	0.553447	0.000713
B	-1.884921	0.790500	-0.000810
C	-0.453173	0.419565	0.000325

A7

E=-180.16705 a.u.

C	1.997629	-0.578988	0.000064
H	2.432666	-0.968516	0.917424
H	2.433147	-0.969186	-0.916777
C	-1.747983	-0.707964	0.000026
H	-2.730653	-0.224900	-0.000204
H	-1.664510	-1.343406	-0.885577
H	-1.664699	-1.342973	0.885963
C	-0.699782	0.332925	-0.000070
C	-0.113222	1.480449	0.000130
B	0.914839	0.338090	-0.000347

A8

E=-180.12592 a.u.

C	1.694499	-0.699798	0.006360
H	1.647649	-1.462826	0.777899
H	2.465864	-0.789266	-0.752308
C	-1.674669	-0.619915	-0.033881
H	-2.666191	-0.172598	-0.149638
H	-1.486773	-1.283191	-0.886046
H	-1.674866	-1.237307	0.871103
C	-0.646075	0.441528	0.023234
B	0.102635	1.637977	0.037330
C	0.826435	0.337403	-0.003657

A9

E=-180.20828 a.u.

C	-2.733315	0.005312	0.000035
H	-3.287132	0.939521	0.000037
H	-3.297007	-0.922999	0.000050
C	-0.130754	-0.008409	-0.000062
C	-1.414217	-0.001734	-0.000008
B	1.235724	-0.016217	-0.000073
C	2.765097	0.000596	0.000026

H	3.188752	-0.478088	0.890257
H	3.188974	-0.476876	-0.890745
H	3.106931	1.044941	0.000812

A10

E=-180.20735 a.u.

C	-2.890802	-0.000249	0.000042
H	-3.475464	-0.917689	0.000075
H	-3.476571	0.916477	0.000089
C	-0.039137	0.000791	-0.000136
C	2.638459	-0.001774	0.000815
H	3.011172	1.013888	-0.176237
H	3.041755	-0.347524	0.959139
H	3.031974	-0.643809	-0.795315
B	-1.498348	0.000494	-0.000266
C	1.184626	-0.002737	0.001542

TS_{A1-A3}

E=-180.12248 a.u.

C	-1.938113	-0.405822	0.000011
H	-2.408257	-0.773132	0.915750
H	-2.408266	-0.773200	-0.915694
C	-0.477833	-0.168450	-0.000021
C	-1.347621	0.977668	-0.000004
B	0.898811	-0.164233	-0.000009
C	2.415504	-0.022970	0.000010
H	2.680000	1.042641	-0.000064
H	2.865425	-0.478793	0.889351
H	2.865417	-0.478914	-0.889274

TS_{A3-A9}

E=-180.09593 a.u.

C	-2.107837	0.560684	0.000213
H	-2.339230	1.091975	0.926298
H	-2.350404	1.078594	-0.930581
C	-0.305026	-0.451854	-0.003983
C	-1.633326	-0.724841	0.006673
B	1.004991	-0.039743	-0.016315
C	2.527012	0.179894	-0.002106
H	2.901358	-0.052599	1.005254
H	2.836818	1.203750	-0.237581
H	3.041566	-0.506302	-0.686596

TS_{A1-A4}

E=-180.11911 a.u.

C	2.038035	-0.452021	-0.000002
H	2.601561	-0.517592	-0.929864
H	2.601576	-0.517588	0.929851
C	0.718363	-0.245794	0.000007
C	0.332595	1.281035	-0.000002
B	-0.664701	0.188365	0.000000
C	-2.142679	-0.341434	-0.000004
H	-2.675414	0.037868	-0.879369
H	-2.206796	-1.432815	-0.000165
H	-2.675304	0.037591	0.879550

TS_{A4-A9}

E=-180.17473 a.u.

C	-1.964207	-0.678429	-0.005665
H	-2.150548	-1.280909	0.877192
H	-2.556722	-0.867439	-0.895092
C	-1.058193	0.295193	0.010940
C	-0.205573	1.305632	0.032153
B	0.875926	0.409889	-0.012516
C	2.085731	-0.525048	-0.015102
H	2.960025	-0.016917	-0.437685
H	2.338598	-0.850104	1.000579
H	1.882468	-1.418166	-0.616370

1

E=-2011.13769 a.u.

Cl	0.547059	-0.277092	2.384148
Cl	3.257943	-0.062491	0.003343
Cl	0.561459	0.262278	-2.380556
C	-1.893001	2.344709	-0.849437
H	-2.674738	3.086073	-0.658193
H	-1.751133	2.277108	-1.936607
C	-1.972728	-2.273596	0.854376
H	-1.818642	-2.202330	1.939729
H	-2.783108	-2.986533	0.675239
B	-0.549707	2.808649	-0.210448
B	-0.651659	-2.789263	0.208615
C	-3.681730	0.706728	-0.220929
H	-4.485874	1.387529	-0.454724
C	-3.704191	-0.577893	0.216357
H	-4.531604	-1.231187	0.447508
Sc	0.887768	-0.016451	0.001865
C	1.705761	3.404728	0.824988
H	2.593573	3.587565	0.221922
H	1.861632	3.457342	1.901335
C	1.578230	-3.461755	-0.835469
H	2.460412	-3.679093	-0.235550
H	1.729498	-3.515363	-1.912420
C	-1.524559	0.027499	0.000548
N	-2.382830	-0.969496	0.338207
N	-2.347460	1.053314	-0.339001
C	0.678112	-2.384874	-0.329030
C	0.258678	-3.776459	-0.296726
C	0.766006	2.358868	0.325288
C	0.397068	3.764531	0.288274

2

E=-817.89160 a.u.

Ti	0.003370	0.233606	-0.002206
C	-2.253443	0.248659	-0.407277
C	-3.680878	0.267445	-0.645687
B	-3.200941	-0.667871	0.336613
C	-2.868519	1.189110	-1.413514
H	-2.672993	0.975572	-2.463537
H	-2.873958	2.246192	-1.150849
C	-3.318153	-1.781110	1.396104
H	-4.029053	-1.495355	2.178788
H	-3.690985	-2.703907	0.937672
H	-2.347637	-1.986613	1.854668
F	0.112697	-1.023531	1.307914
F	-0.560276	1.501990	1.172183

F	0.573022	1.500376	-1.175558
F	-0.110180	-1.018733	-1.313845
C	2.257673	0.243992	0.412916
C	3.684150	0.251900	0.655048
B	3.202202	-0.673549	-0.334556
C	2.875320	1.173449	1.427195
H	2.675405	0.953779	2.475132
H	2.888233	2.232318	1.172123
C	3.294172	-1.779792	-1.403037
H	2.817723	-1.447107	-2.330840
H	4.328983	-2.063442	-1.612441
H	2.744543	-2.666487	-1.069192

3

E=-1707.29620 a.u.

Cl	2.793451	0.000156	0.029797
Cl	0.360664	-2.148511	-0.336764
C	-3.031466	0.000027	1.765970
H	-2.636282	0.880291	2.283890
H	-4.121371	-0.000386	1.851731
H	-2.635577	-0.879793	2.284115
B	-2.577329	-0.000011	0.297241
C	-1.600987	-0.000101	-2.092805
H	-1.367397	-0.924508	-2.620571
H	-1.367415	0.924286	-2.620617
C	-1.308668	-0.000051	-0.594070
C	-2.660933	-0.000083	-1.122337
V	0.621852	-0.000025	0.270828
Cl	0.360416	2.148474	-0.336850
O	0.322175	-0.000002	1.788818

4

E=-1366.95387 a.u.

C	-1.103351	0.950595	0.741624
C	-2.075833	1.635905	1.620551
B	-2.584252	0.480849	0.985091
C	-0.769962	2.234521	1.504528
H	-0.642716	3.126532	0.892867
H	-0.074021	2.146823	2.338830
C	-3.590800	-0.618301	0.589435
H	-3.293936	-1.586625	1.007160
H	-4.596845	-0.382636	0.948288
H	-3.614464	-0.740740	-0.498017
Cl	0.852022	1.597454	-1.757455
Cl	-0.840146	-1.570901	-1.786850
C	1.097248	-0.960388	0.735115
C	2.065973	-1.658525	1.607841
B	2.578985	-0.497671	0.986717
C	0.758364	-2.251712	1.482443
H	0.629744	-3.136489	0.860638
H	0.061163	-2.171403	2.316440
C	3.589441	0.602870	0.605315
H	3.284854	1.571151	1.017347
H	4.590746	0.368846	0.978179
H	3.628354	0.724581	-0.481833
Cr	0.001045	0.004287	-0.512787

5

E=-3606.26164 a.u.

B	-0.583539	1.102496	2.405393
B	1.531139	1.993773	1.629583
Mn	-0.017643	0.258545	-0.437263
C	-1.655933	-1.130211	1.678567
C	3.019344	0.953278	-0.183389
H	0.607653	2.554173	3.595411
H	-0.179530	3.216963	2.144365
C	-4.033159	-1.806910	1.222288
C	-2.712515	-0.823744	-0.577133
H	-4.106395	-2.132976	2.257578
C	-3.830136	-0.963134	-1.424396
C	-5.015050	-1.514004	-0.956568
H	-3.725985	-0.629100	-2.451930
H	-5.861898	-1.611082	-1.630841
C	2.371849	-1.417311	-0.564880
C	4.667492	-0.951273	0.096166
C	2.693689	-2.784026	-0.625729
H	5.431875	-0.229440	0.374622
C	3.978991	-3.220832	-0.323968
H	1.915073	-3.480765	-0.921140
H	4.207071	-4.282272	-0.375007
Br	-0.456884	2.507763	-1.171683
O	-1.592802	-0.338355	-1.110413
O	1.136297	-1.036427	-0.917607
H	-1.205554	-2.075875	1.990518
H	3.323057	1.535662	-1.057217
C	-1.449154	-0.002591	2.583816
C	-0.668257	-0.028708	1.346097
C	1.618873	1.209748	0.314869
C	2.787839	1.702042	1.045210
C	0.337182	2.339839	2.557731
C	3.380436	-0.497170	-0.197294
C	-2.837647	-1.238466	0.773271
C	-5.125634	-1.943510	0.370711
H	-6.052728	-2.374222	0.736676
C	4.974460	-2.309206	0.039913
H	5.977404	-2.652370	0.275052

6

E=-621.85477 a.u.

B	1.516753	2.234834	-0.146819
C	-0.091489	2.035654	-2.142143
H	-0.976650	2.657071	-2.277188
H	0.082034	1.304217	-2.932358
C	2.448220	2.291683	1.080227
H	2.782162	1.284496	1.349504
H	3.328079	2.905097	0.864715
H	1.939212	2.716171	1.951590
Fe	-0.765610	0.181665	0.214690
C	-0.124849	0.452201	1.820963
O	0.203453	0.587590	2.919968
I	1.268227	-1.417758	-0.299364
C	-2.257237	-0.191484	-1.286868
H	-2.096670	-0.120064	-2.353282
C	-2.083902	-1.358012	-0.500479
H	-1.721928	-2.311053	-0.860228
C	-2.363668	-1.043499	0.854703

H	-2.299867	-1.722915	1.693460
C	-2.654071	0.865227	-0.409958
H	-2.862757	1.889503	-0.688725
C	-2.725548	0.344026	0.907558
H	-3.001572	0.898958	1.794638
C	0.208814	1.553245	-0.713510
C	1.028128	2.557878	-1.424401

7

E=-845.04567 a.u.

B	-3.003319	-0.096066	0.525709
C	-2.344611	2.028346	-0.805787
H	-2.378558	2.067769	-1.894232
H	-2.039718	2.952053	-0.314676
C	-3.308752	-1.382177	1.307468
H	-3.787510	-1.133747	2.261500
H	-4.021362	-1.997248	0.745630
H	-2.421017	-1.984758	1.512427
B	3.004110	0.107272	0.526139
C	2.348329	-2.036184	-0.775967
H	2.379844	-2.088954	-1.863926
H	2.047057	-2.954536	-0.272750
C	3.308020	1.400411	1.296801
H	3.630790	1.157448	2.316056
H	4.138524	1.932525	0.819456
H	2.452919	2.077175	1.360644
Co	-0.000049	-0.001981	-0.168025
C	0.008951	0.052229	1.642117
C	-0.593116	-1.486064	-1.053690
C	0.582390	1.426677	-1.144657
O	0.013116	0.085848	2.785812
O	0.941332	2.315609	-1.767984
O	-0.958322	-2.408788	-1.621772
C	3.229372	-1.135839	-0.101370
C	1.836446	-0.711812	-0.162641
C	-1.835405	0.710439	-0.177253
C	-3.227060	1.138702	-0.118547

8

E=-576.10762 a.u.

C	-1.164348	0.000483	0.552689
C	-2.608816	0.000692	0.872159
B	-2.279332	-0.000204	-0.511043
C	-1.691176	0.001315	1.983734
H	-1.549699	0.917771	2.556223
H	-1.549755	-0.914545	2.557194
C	-2.552565	-0.001085	-2.033395
H	-2.104673	-0.882373	-2.505450
H	-3.624331	-0.000702	-2.251101
H	-2.103736	0.879065	-2.506660
C	1.525735	-1.520000	-0.127156
C	1.526145	1.519629	-0.128459
O	2.139913	-2.484387	-0.268651
O	2.140589	2.483741	-0.270697
Ni	0.638392	0.000027	0.082227

9

E=-493.60946 a.u.

C	1.670636	-0.320307	-0.031529
C	2.994964	0.289583	-0.092834
B	1.888612	1.196603	-0.008178
C	2.920017	-1.159107	-0.125833
H	3.104997	-1.674071	-1.067750
H	3.210981	-1.720843	0.760968
C	1.203326	2.576919	0.072877
H	0.736062	2.711064	1.054882
H	1.918418	3.389699	-0.082171
H	0.403162	2.661270	-0.669383
Cu	-0.200320	-0.691716	0.082208
C	-2.106840	-1.039020	0.211163
H	-2.295447	-2.020600	-0.242916
H	-2.373484	-1.094682	1.275093
C	-2.853245	0.032007	-0.487264
C	-3.487615	1.087522	0.058089
H	-3.989430	1.828864	-0.557953
H	-2.871563	-0.045071	-1.578366
H	-3.524923	1.235545	1.136440