Supporting information for

Neutral and Ionic Reaction Mechanisms for Allylation of Aldehydes by Bipyridine *N,N'*-Dioxides

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Contents

I General methods

All solvents unless otherwise stated were used as obtained. THF was distilled from sodium and benzophenone, and dichloromethane from CaH_2 under Ar. All other reagents were obtained from commercial sources. Bis(3-phenyltetrahydroisoquinoline) *N,N'*-dioxide **1** was prepared and resolved into enantiomers according the previously reported method.[1] All reactions were carried out under an argon atmosphere using Schlenk-tube technique.

II. Conductivity measurements by CCD (300kHz/10V)

The test solution conductivity was measured using a contactless conductivity detector (CCD). This approach fully eliminates any interfering interactions of the electrode surface with the solution. (At present, CCDs are very popular for detection in separation methods[2] and the fundamentals of the method can be found elsewhere.[3])

The detection cell used in this work consisted of two 5 mm long stainless steel tubular electrodes (prepared from an injection syringe needle) placed on the outside of the PTFE tubing (i.d. 1.5 mm, o.d. 2 mm) with a gap between them of 2.5 mm. A sine-wave signal from a GFG 3015 (Instek) function generator, peak-to-peak voltage of 20 V and frequency of 300 kHz, was fed to one of the electrodes and the signal, the current whose magnitude depends on the conductivity of the detection space between the electrodes, is measured at the other electrode. The detector electronics was based on the scheme described in ref. 4; the electronics converts the alternating current to a d. c. voltage. The voltage signal cannot be transferred into conductivity units because its magnitude is not solely determined by the solution conductivity but, to a certain extent, also by the solution permittivity which depends on the actual solution composition. Therefore, the data presented can be related to the conductivity in the sense that a higher voltage indicates a higher conductivity (or a higher content of the ionic species) in the solution.

The test solution was aspirated into the detection cell using a hypodermic syringe from the vessel closed by a septum. All the measurements were carried out under laboratory temperature. A block scheme of the apparatus is shown in Fig. 1.

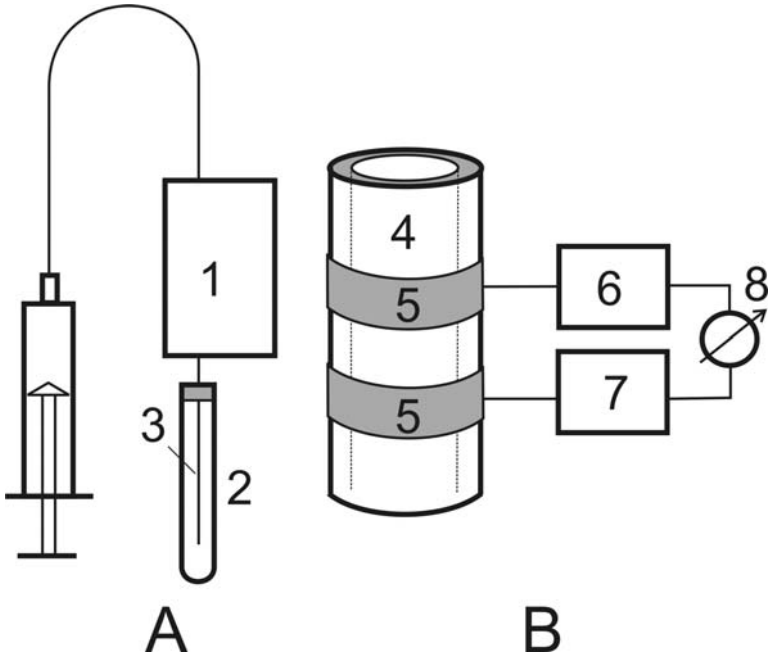


Fig. 1. A block scheme of the apparatus for contactless measurement of conductivity (A) and a detailed scheme of the detection cell and its connection to the detector electronics (B). 1 – the detector in the faradaic cage, 2 – vessel with sample closed with the septum, 3 – sampling needle, 4 – PTFE tubing, 5 – conductometric electrodes, 6 – sine-wave generator, 7 – electronics, 8 – voltmeter.

All the measurements were performed under the same conditions, stated values are relative. Stock solutions of allyltrichlorosilane in corresponding anhydrous solvents were prepared separately to avoid water contamination and were used for preparation of **1**/allyltrichlorosilane solutions (Table 1, in the text).

Entry 1. **1** (5 mg, 0.0112 mmol) dissolved in anhydrous CH_3CN (1 mL), measured background conductivity related to voltage (1560 mV).

Entry 3. Allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in anhydrous CH_3CN (1 mL), measured background conductivity related to voltage (1510 mV).

Entry 3. **1** (5 mg, 0.0112 mmol) and allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in CH_3CN (1 mL), measured conductivity related to voltage (1780 mV).

Entry 4. Allyltrichlorosilane (3.92 mg, 0.0224 mmol) dissolved in anhydrous CH_3CN (1 mL), measured background conductivity related to voltage (1560 mV).

Entry 5. **1** (10 mg, 0.0224 mmol) and allyltrichlorosilane (3.92 mg, 0.0224 mmol) dissolved in CH_3CN (1 mL), measured conductivity related to voltage (2100 mV).

Entry 6. Allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in anhydrous CH_2Cl_2 (1 mL), measured background conductivity related to voltage (188 mV).

Entry 7. **1** (5 mg, 0.0112 mmol) and allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in CH_2Cl_2 (1 mL), measured conductivity related to voltage (458 mV).

Entry 8. Allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in anhydrous PhCl (1 mL), measured background conductivity related to voltage (55 mV).

Entry 9. **1** (5 mg, 0.0112 mmol) and allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in PhCl (1 mL), measured conductivity related to voltage (57 mV).

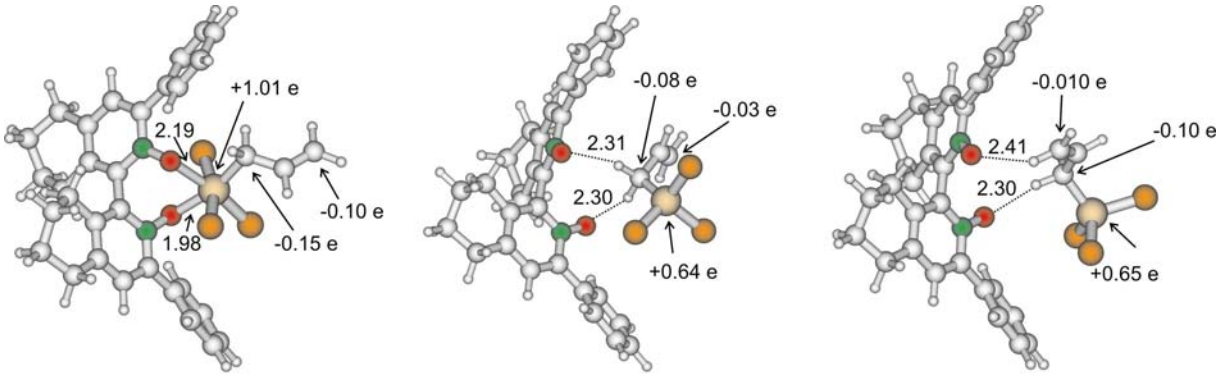
Entry 10. Allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in anhydrous EtOAc (1 mL), measured background conductivity related to voltage (62 mV).

Entry 11. **1** (5 mg, 0.0112 mmol) and allyltrichlorosilane (1.96 mg, 0.0112 mmol) dissolved in EtOAc (1 mL), measured conductivity related to voltage (63 mV).

III Calculations

Geometries, total energies, and zero-point energies (ZPEs) of the optimized structures of the studied neutral and cationic complexes between **1** and $(C_3H_5)SiCl_3$. Further, SCRF energies obtained by single-point PCM calculations are given for the following solvents: acetonitrile (ACN), dichloromethane (DCM), chlorbenzene (PhCl), and toluene (TOL).

Three most stable arrangements found for the complex [1•$SiCl_3(C_3H_5)$]



2 **2a** **2b**

Note that although the isomers **2**a and **2**b lie lower in energy than the isomer **2** considered in the reaction mechanism; however, the mode of binding leads to a much smaller polarization of the allyl group and these forms will most probably not be reactive. It is also supported by the fact that such a non-specific binding would most probably not lead to the high ees as observed in the experiment. Other optimized geometries of the same complex with higher energies are listed in the following table as isomers **2**c – **2**g in that isomers **2**c – **2**e have similar geometry to the isomer **2** only the allyl group has slightly different orientation, whereas the binding in isomers **2**f and **2**g does not contain the direct O-Si bonds as it is the case for **2**a or **2**b. The conformational search was performed manually and we tried to start the optimization with all possible orientations and positions of the allyl group with respect to the ligand **1**.

Isomer	Total energy/Hartree ZPE/Hartree PCM energy/Hartree	Geometry Center Number / Atomic Number / Atomic Type / Coordinates (Angstroms) X Y Z
2	E_{tot}: -3207.510633 ZPE: 0.592464 ACN: -3207.556904 DCM: -3207.549563	1 6 0 3.825451 -0.539714 1.793582 2 6 0 3.836250 -0.209055 0.428766 3 6 0 4.859060 -0.712327 -0.390043 4 6 0 5.856118 -1.524165 0.145991 5 6 0 5.848313 -1.835599 1.506080 6 6 0 4.831543 -1.341510 2.325731 7 6 0 2.849325 0.725859 -0.149106

PhCl: -3207.54374

TOL:-3207.530282

8	6	0	3.216249	1.747574	-1.019826
9	6	0	2.296943	2.635410	-1.575688
10	6	0	0.953942	2.548254	-1.164117
11	6	0	0.613650	1.553934	-0.244060
12	7	0	1.525060	0.636669	0.185643
13	6	0	2.756917	3.648873	-2.603859
14	6	0	1.742755	4.771083	-2.851243
15	6	0	0.337903	4.183101	-3.010333
16	6	0	-0.104810	3.488805	-1.715309
17	6	0	-0.748256	1.438478	0.351208
18	6	0	-1.230389	2.338879	1.301650
19	6	0	-2.581404	2.231256	1.687892
20	6	0	-3.374315	1.271058	1.066533
21	6	0	-2.864292	0.337716	0.164983
22	7	0	-1.531785	0.427580	-0.117968
23	6	0	-0.313093	3.385979	1.910506
24	6	0	-0.859061	3.952710	3.227789
25	6	0	-2.327045	4.358812	3.070721
26	6	0	-3.181933	3.127388	2.751295
27	6	0	-3.732590	-0.652379	-0.500721
28	6	0	-3.627979	-0.915825	-1.875504
29	6	0	-4.546050	-1.759763	-2.493435
30	6	0	-5.560446	-2.365091	-1.750586
31	6	0	-5.656938	-2.123855	-0.379242
32	6	0	-4.752374	-1.268275	0.242338
33	8	0	-0.933371	-0.484157	-0.893680
34	14	0	0.051106	-2.010529	-0.097277
35	17	0	-1.217859	-3.406736	-1.134042
36	8	0	1.075831	-0.360798	0.920982
37	17	0	1.373824	-1.618688	-1.884738
38	6	0	1.336732	-3.125698	0.835592
39	17	0	-1.276057	-1.865530	1.743065
40	1	0	2.936518	3.111729	-3.545878
41	1	0	2.031593	5.339522	-3.741129
42	1	0	-0.386343	4.962567	-3.268372
43	1	0	-1.035041	2.936713	-1.881271
44	1	0	4.266991	1.831491	-1.274874
45	1	0	-4.434121	1.221005	1.288590
46	1	0	0.680365	2.954438	2.065642
47	1	0	-0.247555	4.807376	3.534703
48	1	0	-2.700053	4.838793	3.981006
49	1	0	-3.299858	2.523569	3.662185
50	1	0	-0.335858	4.258155	-0.965819
51	1	0	0.334902	3.460117	-3.835786
52	1	0	1.751372	5.476286	-2.009299
53	1	0	3.728064	4.057142	-2.301080
54	1	0	-0.179245	4.212755	1.199790
55	1	0	-0.770477	3.197711	4.019200
56	1	0	-2.418538	5.097624	2.263364
57	1	0	-4.195126	3.417435	2.450563

		58	1	0	3.024140	-0.179291	2.426515
		59	1	0	4.814599	-1.590113	3.382366
		60	1	0	6.623552	-2.471039	1.923662
		61	1	0	6.630792	-1.922634	-0.501821
		62	1	0	4.847351	-0.499738	-1.453992
		63	1	0	-2.822918	-0.475834	-2.449984
		64	1	0	-4.455809	-1.958464	-3.556614
		65	1	0	-6.264163	-3.034866	-2.235803
		66	1	0	-6.427739	-2.611492	0.209418
		67	1	0	-4.806677	-1.109443	1.314318
		68	6	0	0.905144	-4.534510	1.087421
		69	1	0	2.272013	-3.102053	0.271162
		70	1	0	1.499703	-2.610165	1.787380
		71	6	0	1.549727	-5.621856	0.656427
		72	1	0	-0.001903	-4.656967	1.677519
		73	1	0	1.189621	-6.622720	0.877699
		74	1	0	2.453019	-5.549340	0.054938
2a	E_{tot}: -3207.5401055 ZPE: 0.591762 ACN: -3207.559016 DCM: -3207.555542 PhCl: -3207.55247 TOL: -3207.547275	1	6	0	-4.054498	1.252702	1.707650
		2	6	0	-3.924043	1.030522	0.325583
		3	6	0	-4.577203	1.904752	-0.561151
		4	6	0	-5.349385	2.961950	-0.083795
		5	6	0	-5.484569	3.163596	1.289890
		6	6	0	-4.835046	2.305539	2.179406
		7	6	0	-3.176289	-0.116038	-0.239637
		8	6	0	-3.652115	-0.835460	-1.329072
		9	6	0	-2.948894	-1.888892	-1.913303
		10	6	0	-1.696937	-2.217545	-1.372610
		11	6	0	-1.234532	-1.511761	-0.256455
		12	7	0	-1.964707	-0.492537	0.310499
		13	6	0	-3.533619	-2.636045	-3.095037
		14	6	0	-2.871521	-4.000122	-3.315646
		15	6	0	-1.349116	-3.840630	-3.311245
		16	6	0	-0.842814	-3.328624	-1.954988
		17	6	0	0.055384	-1.825229	0.421023
		18	6	0	0.129249	-2.506018	1.640556
		19	6	0	1.391117	-2.817839	2.168248
		20	6	0	2.514500	-2.400534	1.455147
		21	6	0	2.438751	-1.696045	0.259105
		22	7	0	1.184618	-1.426935	-0.257757
		23	6	0	-1.152577	-2.907029	2.346965
		24	6	0	-0.927498	-3.403303	3.782577
		25	6	0	0.280988	-4.339417	3.866817
		26	6	0	1.550611	-3.579246	3.468703
		27	6	0	3.653595	-1.239246	-0.454490
		28	6	0	3.788897	-1.306753	-1.852404
		29	6	0	4.988709	-0.945966	-2.460776
		30	6	0	6.067071	-0.496956	-1.696268
		31	6	0	5.938885	-0.410781	-0.310058
		32	6	0	4.744449	-0.780268	0.304539
		33	8	0	1.055259	-0.808189	-1.387857

		34	14	0	1.462916	3.371378	0.205095
		35	17	0	2.819173	3.981887	-1.235532
		36	8	0	-1.501732	0.106253	1.359762
		37	6	0	0.123183	2.280282	-0.499042
		38	17	0	0.666130	5.083535	1.069488
		39	17	0	2.522922	2.370076	1.681412
		40	1	0	-3.404290	-2.025329	-4.000540
		41	1	0	-3.216350	-4.432781	-4.260871
		42	1	0	-0.854407	-4.788526	-3.548215
		43	1	0	0.178524	-2.952867	-2.063261
		44	1	0	-4.628051	-0.563858	-1.717753
		45	1	0	3.503830	-2.647095	1.826004
		46	1	0	-1.821017	-2.041530	2.359098
		47	1	0	-1.835157	-3.900764	4.140613
		48	1	0	0.391529	-4.744858	4.878244
		49	1	0	1.805374	-2.866643	4.266689
		50	1	0	-0.805561	-4.160425	-1.237765
		51	1	0	-1.062020	-3.131546	-4.098588
		52	1	0	-3.173435	-4.693693	-2.519284
		53	1	0	-4.615888	-2.744137	-2.956472
		54	1	0	-1.650500	-3.691923	1.760447
		55	1	0	-0.759672	-2.542740	4.443076
		56	1	0	0.133420	-5.195509	3.194806
		57	1	0	2.405991	-4.260449	3.388355
		58	1	0	-3.532844	0.606431	2.399929
		59	1	0	-4.930098	2.460154	3.250172
		60	1	0	-6.082902	3.988846	1.664677
		61	1	0	-5.835912	3.632425	-0.786038
		62	1	0	-4.453527	1.770706	-1.631226
		63	1	0	2.948934	-1.630332	-2.451239
		64	1	0	5.078346	-1.009700	-3.541301
		65	1	0	6.995715	-0.205958	-2.178380
		66	1	0	6.763227	-0.044829	0.294583
		67	1	0	4.645476	-0.684984	1.381186
		68	6	0	-0.765039	2.985831	-1.486276
		69	1	0	0.614487	1.407826	-0.951837
		70	1	0	-0.452864	1.901658	0.358572
		71	6	0	-0.778508	2.746526	-2.799101
		72	1	0	-1.433514	3.741249	-1.075538
		73	1	0	-1.440955	3.290496	-3.465981
		74	1	0	-0.131229	1.998005	-3.248304
2b	E_{tot}: -3207.5388008 ZPE: 0.591901 ACN: -3207.557644 DCM: -3207.554478 PhCl: -3207.551818 TOL: -3207.546159	1	6	0	-3.027425	-0.461188	4.033873
		2	6	0	-2.747813	-0.360010	2.547958
		3	6	0	-1.926185	0.643735	2.013317
		4	6	0	-1.259116	1.682905	2.895321
		5	6	0	-1.338367	1.353256	4.393066
		6	6	0	-2.729112	0.843402	4.780262
		7	6	0	-3.310300	-1.278359	1.661968
		8	6	0	-3.096375	-1.242401	0.288560
		9	7	0	-2.311899	-0.222476	-0.220189

		10	6	0	-1.736718	0.696961	0.628598
		11	6	0	-0.943766	1.764868	-0.042888
		12	6	0	-1.537748	2.819499	-0.744987
		13	6	0	-0.718109	3.816113	-1.293806
		14	6	0	0.660586	3.684014	-1.132265
		15	6	0	1.250388	2.621827	-0.456942
		16	7	0	0.421289	1.665929	0.102014
		17	6	0	-3.049132	2.870407	-0.871850
		18	6	0	-3.543500	3.927824	-1.869989
		19	6	0	-2.770664	5.241170	-1.723329
		20	6	0	-1.289665	5.005773	-2.037834
		21	8	0	0.913491	0.681008	0.783130
		22	8	0	-2.111604	-0.111474	-1.491794
		23	6	0	1.455615	-2.579016	0.168275
		24	6	0	0.767958	-3.342096	-0.932866
		25	6	0	-0.086620	-2.809536	-1.808162
		26	14	0	3.314510	-2.497991	-0.029951
		27	17	0	4.197751	-1.747675	1.691216
		28	17	0	4.099953	-4.401754	-0.321861
		29	17	0	3.899488	-1.335474	-1.631747
		30	1	0	-1.176575	4.835899	-3.118616
		31	1	0	-3.175846	6.009337	-2.390677
		32	1	0	-4.617712	4.086484	-1.727133
		33	1	0	-3.399456	1.882303	-1.182527
		34	6	0	2.720872	2.509287	-0.324462
		35	1	0	1.319569	4.452255	-1.522965
		36	6	0	-3.685748	-2.254664	-0.617991
		37	1	0	-3.968884	-2.051707	2.043231
		38	1	0	-0.211560	1.765379	2.592434
		39	1	0	-1.070383	2.241962	4.974273
		40	1	0	-2.797653	0.678109	5.860812
		41	1	0	-2.407494	-1.264684	4.458082
		42	1	0	-3.480897	3.068950	0.119078
		43	1	0	-3.415433	3.550495	-2.892969
		44	1	0	-2.877389	5.621169	-0.698355
		45	1	0	-0.694157	5.897396	-1.808833
		46	1	0	-1.726938	2.659794	2.708696
		47	1	0	-0.594620	0.583405	4.636574
		48	1	0	-3.484453	1.598969	4.525366
		49	1	0	-4.068069	-0.770516	4.187365
		50	1	0	1.287443	-3.056051	1.144624
		51	1	0	1.096407	-1.543853	0.241224
		52	1	0	1.006503	-4.403117	-0.997549
		53	1	0	-0.548393	-3.425284	-2.574690
		54	1	0	-0.381453	-1.763420	-1.785551
		55	6	0	3.351380	2.124642	0.871223
		56	6	0	4.741043	2.130179	0.966049
		57	6	0	5.526661	2.499727	-0.126935
		58	6	0	4.911846	2.867367	-1.323791
		59	6	0	3.522106	2.874163	-1.420415

		60	1	0	2.749059	1.812465	1.713120
		61	1	0	5.212041	1.832752	1.897959
		62	1	0	6.609849	2.489189	-0.049775
		63	1	0	5.512122	3.138980	-2.187006
		64	1	0	3.052067	3.139416	-2.362436
		65	6	0	-4.226631	-1.933037	-1.875394
		66	6	0	-4.845050	-2.914352	-2.646861
		67	6	0	-4.923708	-4.232280	-2.192990
		68	6	0	-4.376248	-4.566222	-0.954137
		69	6	0	-3.764299	-3.586870	-0.174999
		70	1	0	-4.145611	-0.919552	-2.242631
		71	1	0	-5.263344	-2.646912	-3.612880
		72	1	0	-5.398947	-4.994052	-2.804090
		73	1	0	-4.414815	-5.590942	-0.596608
		74	1	0	-3.318142	-3.862368	0.775471
2c	E_{tot}: -3207.510514 ZPE: 0.592558 ACN: -3207.556775 DCM: -3207.549107 PhCl: -3207.543513 TOL: -3207.530097	1	6	0	3.662154	-1.333696	1.733789
		2	6	0	3.767785	-0.990532	0.376765
		3	6	0	4.736630	-1.622709	-0.419170
		4	6	0	5.591071	-2.572027	0.133384
		5	6	0	5.495256	-2.892830	1.488351
		6	6	0	4.530535	-2.272310	2.283105
		7	6	0	2.958941	0.093861	-0.212263
		8	6	0	3.516102	1.043355	-1.067919
		9	6	0	2.779760	2.088313	-1.618248
		10	6	0	1.443593	2.259126	-1.204545
		11	6	0	0.917145	1.335813	-0.300986
		12	7	0	1.639651	0.254041	0.099958
		13	6	0	3.424088	3.006465	-2.636336
		14	6	0	2.649376	4.308816	-2.865808
		15	6	0	1.155323	4.012016	-3.021070
		16	6	0	0.590099	3.399895	-1.732547
		17	6	0	-0.429602	1.499015	0.317321
		18	6	0	-0.692563	2.451385	1.303798
		19	6	0	-2.025054	2.612302	1.727893
		20	6	0	-3.010633	1.847468	1.107670
		21	6	0	-2.723394	0.862925	0.166011
		22	7	0	-1.408111	0.681394	-0.163351
		23	6	0	0.435682	3.270035	1.908799
		24	6	0	0.049541	3.909154	3.249499
		25	6	0	-1.308911	4.607248	3.142151
		26	6	0	-2.403748	3.581561	2.829150
		27	6	0	-3.786938	0.086812	-0.503129
		28	6	0	-3.770190	-0.130747	-1.891058
		29	6	0	-4.857324	-0.736071	-2.515778
		30	6	0	-5.963246	-1.147068	-1.767912
		31	6	0	-5.974426	-0.957796	-0.385658
		32	6	0	-4.894863	-0.342348	0.243594
		33	8	0	-1.032658	-0.313251	-0.948988
		34	14	0	-0.138254	-2.050593	-0.032658
		35	6	0	-1.397953	-3.179010	-0.975472

		36	8	0	0.993156	-0.656714	0.834692
		37	17	0	1.168543	-1.882145	-1.885567
		38	17	0	1.051373	-3.600286	0.912377
		39	17	0	-1.395307	-1.644013	1.777492
		40	1	0	3.489793	2.453053	-3.583797
		41	1	0	3.041154	4.818006	-3.752039
		42	1	0	0.598926	4.923588	-3.262216
		43	1	0	-0.431948	3.045906	-1.897729
		44	1	0	4.566994	0.938142	-1.311998
		45	1	0	-4.052803	2.003816	1.363251
		46	1	0	1.320649	2.638423	2.033306
		47	1	0	0.829817	4.615649	3.550723
		48	1	0	-1.551849	5.134004	4.070553
		49	1	0	-2.615827	2.992939	3.732941
		50	1	0	0.520738	4.186980	-0.969293
		51	1	0	1.004281	3.317415	-3.857130
		52	1	0	2.801483	4.989357	-2.017387
		53	1	0	4.458201	3.210630	-2.336233
		54	1	0	0.724837	4.066342	1.209133
		55	1	0	0.003581	3.136030	4.026807
		56	1	0	-1.269258	5.366097	2.349192
		57	1	0	-3.344794	4.078698	2.567034
		58	1	0	2.894160	-0.880154	2.347042
		59	1	0	4.439956	-2.531773	3.333085
		60	1	0	6.159879	-3.635368	1.919829
		61	1	0	6.321769	-3.069555	-0.496709
		62	1	0	4.789008	-1.400270	-1.479892
		63	1	0	-2.905528	0.168398	-2.470543
		64	1	0	-4.837523	-0.892720	-3.589941
		65	1	0	-6.805186	-1.625601	-2.259184
		66	1	0	-6.817900	-1.299277	0.206215
		67	1	0	-4.892602	-0.224067	1.322148
		68	1	0	-0.735255	-3.826065	-1.562218
		69	6	0	-2.311061	-4.024233	-0.147157
		70	1	0	-1.959732	-2.559789	-1.679775
		71	6	0	-3.636364	-4.101385	-0.291596
		72	1	0	-1.828164	-4.639167	0.611047
		73	1	0	-4.238517	-4.757434	0.331394
		74	1	0	-4.166758	-3.509508	-1.033172
2d	E_{tot}: -3207. 5102168 ZPE: 0.592071	1	6	0	3.050724	3.435571	-2.584539
		2	6	0	2.524130	2.451130	-1.560284
		3	6	0	1.183800	2.463215	-1.134568
		4	6	0	0.192874	3.484625	-1.667234
		5	6	0	0.675621	4.160432	-2.957882
		6	6	0	2.123677	4.635656	-2.808476
		7	6	0	3.375594	1.486649	-1.023312
		8	6	0	2.940932	0.492080	-0.153180
		9	7	0	1.618225	0.504599	0.206488
		10	6	0	0.778277	1.492058	-0.216286
		11	6	0	-0.584358	1.474320	0.388502

		12	6	0	-0.980804	2.391058	1.362752
		13	6	0	-2.332893	2.394524	1.758960
		14	6	0	-3.213375	1.527604	1.118604
		15	6	0	-2.794311	0.578801	0.187446
		16	7	0	-1.459892	0.550699	-0.099173
		17	6	0	0.028963	3.342653	1.982106
		18	6	0	-0.455794	3.935320	3.312186
		19	6	0	-1.886598	4.464490	3.178017
		20	6	0	-2.843416	3.312844	2.849191
		21	8	0	-0.951853	-0.392675	-0.904596
		22	8	0	1.101286	-0.448148	0.942622
		23	14	0	-0.165716	-2.054790	-0.195603
		24	17	0	1.220245	-1.679564	-1.942656
		25	6	0	1.035141	-3.365520	0.578494
		26	1	0	-2.994644	2.701590	3.750233
		27	1	0	-2.209158	4.958682	4.099931
		28	1	0	0.228053	4.731508	3.623690
		29	1	0	0.980790	2.822006	2.123623
		30	6	0	-3.754794	-0.302564	-0.504588
		31	1	0	-4.272558	1.569019	1.345271
		32	6	0	3.855904	-0.530665	0.393912
		33	1	0	4.425931	1.487147	-1.293947
		34	1	0	-0.775764	3.003075	-1.834033
		35	1	0	0.011869	4.997372	-3.198391
		36	1	0	2.445753	5.190703	-3.695457
		37	1	0	3.178765	2.897573	-3.534551
		38	1	0	0.231919	4.164348	1.281869
		39	1	0	-0.422655	3.164916	4.093022
		40	1	0	-1.925037	5.221178	2.383123
		41	1	0	-3.834616	3.689030	2.571781
		42	1	0	0.021343	4.258883	-0.906580
		43	1	0	0.607875	3.450947	-3.792229
		44	1	0	2.195674	5.328180	-1.958955
		45	1	0	4.053420	3.765401	-2.288828
		46	6	0	3.843313	-0.881438	1.753982
		47	6	0	4.787139	-1.774868	2.253853
		48	6	0	5.743253	-2.339796	1.407064
		49	6	0	5.751309	-2.008264	0.051992
		50	6	0	4.815857	-1.107180	-0.451943
		51	1	0	3.086778	-0.465003	2.407416
		52	1	0	4.769463	-2.037782	3.307099
		53	1	0	6.469617	-3.045027	1.799828
		54	1	0	6.476805	-2.460386	-0.617280
		55	1	0	4.800768	-0.878160	-1.512476
		56	6	0	-3.684903	-0.518973	-1.889637
		57	6	0	-4.681671	-1.248898	-2.530429
		58	6	0	-5.743102	-1.786275	-1.801016
		59	6	0	-5.807408	-1.591729	-0.420381
		60	6	0	-4.822753	-0.849284	0.224646
		61	1	0	-2.846727	-0.131594	-2.454963

		62	1	0	-4.618092	-1.412087	-3.601556
		63	1	0	-6.509939	-2.367283	-2.304610
		64	1	0	-6.616742	-2.028083	0.156683
		65	1	0	-4.855235	-0.727163	1.302314
		66	17	0	-1.556120	-3.276583	-1.272808
		67	17	0	-1.396901	-1.795535	1.668770
		68	1	0	1.554223	-3.804554	-0.277630
		69	1	0	1.766778	-2.789068	1.152193
		70	6	0	0.429401	-4.439218	1.424786
		71	6	0	0.349619	-5.726714	1.078217
		72	1	0	0.034114	-4.129660	2.389653
		73	1	0	-0.096734	-6.466906	1.736545
		74	1	0	0.715315	-6.083525	0.118328
2e	E_{tot}: -3207.5063907 ZPE: 0.592552 ACN: -3207.552188 DCM: -3207.544883 PhCl: -3207.539045 TOL: -3207.524551	1	6	0	-3.239479	2.716772	3.044157
		2	6	0	-2.656330	1.897292	1.912252
		3	6	0	-1.340713	2.088510	1.453527
		4	6	0	-0.452318	3.178256	2.031843
		5	6	0	-0.947206	3.680049	3.395219
		6	6	0	-2.445258	3.992574	3.345103
		7	6	0	-3.426897	0.916035	1.292659
		8	6	0	-2.917204	0.043424	0.334931
		9	7	0	-1.596509	0.183452	0.001102
		10	6	0	-0.861852	1.240572	0.451562
		11	6	0	0.430640	1.512896	-0.237412
		12	6	0	0.587727	2.559797	-1.147745
		13	6	0	1.885034	2.832091	-1.621610
		14	6	0	2.943175	2.074843	-1.122770
		15	6	0	2.757640	0.994300	-0.265415
		16	7	0	1.474707	0.716834	0.113413
		17	6	0	-0.613210	3.361851	-1.619343
		18	6	0	-0.336815	4.126287	-2.921026
		19	6	0	0.986897	4.890463	-2.827680
		20	6	0	2.150768	3.907917	-2.653900
		21	8	0	1.185083	-0.370979	0.815236
		22	8	0	-1.011111	-0.662819	-0.841295
		23	14	0	0.377584	-2.029409	-0.204814
		24	17	0	-0.807326	-2.159505	1.711431
		25	17	0	-0.732076	-3.552541	-1.277242
		26	1	0	2.345099	3.405912	-3.612192
		27	1	0	1.150463	5.499386	-3.722471
		28	1	0	-1.168661	4.808944	-3.122634
		29	1	0	-1.470282	2.694111	-1.748530
		30	6	0	3.887566	0.195508	0.250082
		31	1	0	3.959969	2.308012	-1.418990
		32	6	0	-3.819315	-0.897641	-0.375332
		33	1	0	-4.464346	0.780560	1.577518
		34	1	0	0.574240	2.809142	2.115675
		35	1	0	-0.372639	4.566224	3.683832
		36	1	0	-2.786218	4.423890	4.291640
		37	1	0	-3.255177	2.080420	3.940412

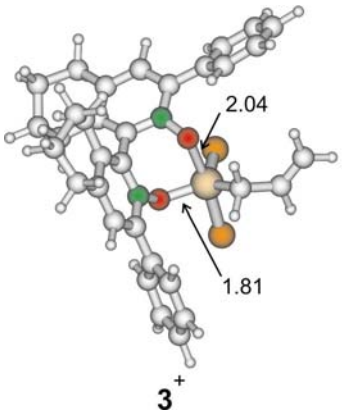
		38	1	0	-0.899410	4.081509	-0.839887
		39	1	0	-0.294527	3.420357	-3.759879
		40	1	0	0.951481	5.582993	-1.975970
		41	1	0	3.076693	4.435822	-2.398110
		42	1	0	-0.415388	4.026809	1.334912
		43	1	0	-0.757878	2.916109	4.159966
		44	1	0	-2.636835	4.744473	2.567859
		45	1	0	-4.287713	2.947597	2.822657
		46	6	0	-4.919212	-0.326682	-1.041443
		47	6	0	-5.847607	-1.135194	-1.692304
		48	6	0	-5.694593	-2.522736	-1.672130
		49	6	0	-4.612982	-3.091747	-1.000537
		50	6	0	-3.674912	-2.289220	-0.352130
		51	1	0	-5.032768	0.753667	-1.064495
		52	1	0	-6.684466	-0.682078	-2.215416
		53	1	0	-6.416733	-3.156502	-2.178702
		54	1	0	-4.486234	-4.169381	-0.980684
		55	1	0	-2.845916	-2.738082	0.175540
		56	6	0	3.981102	-0.148704	1.608639
		57	6	0	5.107872	-0.814587	2.083469
		58	6	0	6.144798	-1.156515	1.212659
		59	6	0	6.051347	-0.829848	-0.140516
		60	6	0	4.931320	-0.154151	-0.620001
		61	1	0	3.167191	0.092668	2.281506
		62	1	0	5.171423	-1.075779	3.135246
		63	1	0	7.015924	-1.686377	1.586007
		64	1	0	6.843586	-1.111677	-0.827063
		65	1	0	4.844000	0.068586	-1.678332
		66	6	0	1.880179	-3.115713	0.367887
		67	17	0	1.449626	-1.310995	-2.056690
		68	6	0	1.621580	-4.215468	1.346799
		69	1	0	2.279248	-3.525890	-0.564178
		70	1	0	2.621922	-2.417779	0.766604
		71	6	0	1.665070	-5.519528	1.061479
		72	1	0	1.382999	-3.910559	2.363756
		73	1	0	1.470535	-6.274859	1.817960
		74	1	0	1.880396	-5.876660	0.057384
2f	E_{tot}: -3207.5368226 ZPE: 0.591594 ACN: -3207.556378 DCM: -3207.553027 PhCl: -3207.549759 TOL: -3207.544234	1	6	0	1.888983	5.116684	-1.624009
		2	6	0	1.743447	3.725550	-1.041743
		3	6	0	0.527786	3.261511	-0.519222
		4	6	0	-0.720430	4.123777	-0.520235
		5	6	0	-0.585348	5.398278	-1.367279
		6	6	0	0.777144	6.065628	-1.164453
		7	6	0	2.836016	2.859563	-1.010956
		8	6	0	2.773143	1.578268	-0.477876
		9	7	0	1.575408	1.156336	0.069925
		10	6	0	0.471059	1.977834	0.037586
		11	6	0	-0.762573	1.422704	0.662224
		12	6	0	-0.926763	1.292600	2.045476
		13	6	0	-2.146109	0.809744	2.542378

		14	6	0	-3.126324	0.451174	1.617548
		15	6	0	-2.953365	0.557812	0.242929
		16	7	0	-1.757613	1.074729	-0.226286
		17	6	0	0.203659	1.702501	2.971529
		18	6	0	-0.009214	1.259750	4.426491
		19	6	0	-1.450508	1.504604	4.880122
		20	6	0	-2.409301	0.666772	4.027703
		21	8	0	-1.561901	1.243663	-1.488068
		22	8	0	1.483618	-0.005595	0.635004
		23	6	0	1.867444	-3.092515	-0.358459
		24	6	0	2.601907	-3.853607	0.708566
		25	6	0	3.482913	-4.830845	0.488007
		26	14	0	0.043885	-3.504027	-0.451879
		27	17	0	-0.925862	-2.246989	-1.765919
		28	17	0	-0.868307	-3.340107	1.405210
		29	17	0	-0.244847	-5.454668	-1.101216
		30	1	0	-2.302622	-0.391974	4.305643
		31	1	0	-1.575089	1.252392	5.938749
		32	1	0	0.700635	1.786626	5.073310
		33	1	0	1.133031	1.270428	2.590554
		34	6	0	-4.005468	0.134589	-0.709335
		35	1	0	-4.086346	0.090534	1.971799
		36	6	0	3.948036	0.675732	-0.488222
		37	1	0	3.795512	3.194833	-1.390818
		38	1	0	-1.548818	3.518924	-0.899080
		39	1	0	-1.400076	6.086384	-1.118036
		40	1	0	0.837455	7.007440	-1.720338
		41	1	0	1.868207	5.046283	-2.721434
		42	1	0	0.315081	2.795411	2.932900
		43	1	0	0.217296	0.189411	4.517336
		44	1	0	-1.694360	2.570534	4.775849
		45	1	0	-3.452285	0.930741	4.239237
		46	1	0	-0.964008	4.394305	0.516579
		47	1	0	-0.703688	5.143942	-2.428653
		48	1	0	0.914515	6.312580	-0.103117
		49	1	0	2.876835	5.516170	-1.365831
		50	1	0	2.285631	-3.295379	-1.351829
		51	1	0	1.918652	-2.008299	-0.181795
		52	1	0	2.371016	-3.567372	1.733603
		53	1	0	3.977037	-5.343146	1.307787
		54	1	0	3.743539	-5.151452	-0.517519
		55	6	0	4.310183	-0.119855	0.613011
		56	6	0	5.470157	-0.890154	0.573908
		57	6	0	6.284114	-0.891573	-0.560527
		58	6	0	5.929718	-0.113817	-1.662814
		59	6	0	4.773082	0.662716	-1.626332
		60	1	0	3.672436	-0.137325	1.486190
		61	1	0	5.734991	-1.498851	1.433163
		62	1	0	7.182371	-1.501367	-0.587983
		63	1	0	6.546642	-0.117483	-2.556570

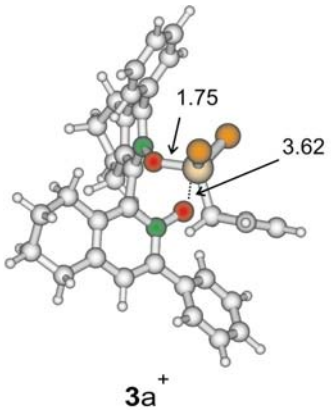
		64	1	0	4.491745	1.246553	-2.497430
		65	6	0	-4.329269	0.864740	-1.866326
		66	6	0	-5.388171	0.463728	-2.677602
		67	6	0	-6.131947	-0.675782	-2.365589
		68	6	0	-5.808498	-1.417833	-1.229613
		69	6	0	-4.756567	-1.015552	-0.409419
		70	1	0	-3.740040	1.732832	-2.127143
		71	1	0	-5.628813	1.043188	-3.564270
		72	1	0	-6.949461	-0.988666	-3.008623
		73	1	0	-6.366133	-2.317214	-0.985643
		74	1	0	-4.493919	-1.614951	0.456690
2g	E_{tot}: -3207.539969 ZPE: 0.591471 ACN: -3207.558376 DCM: -3207.555235 PhCl: -3207.552287 TOL: -3207.547039	1	6	0	3.480471	-1.899475	-1.920070
		2	6	0	3.392151	-1.676375	-0.534693
		3	6	0	4.543281	-1.255660	0.153923
		4	6	0	5.750840	-1.073397	-0.517013
		5	6	0	5.830942	-1.312958	-1.888657
		6	6	0	4.692632	-1.726239	-2.583591
		7	6	0	2.156334	-1.927001	0.242190
		8	6	0	2.187900	-2.523141	1.497205
		9	6	0	1.045953	-2.739106	2.267996
		10	6	0	-0.186551	-2.326991	1.740340
		11	6	0	-0.219126	-1.754241	0.464471
		12	7	0	0.926477	-1.560455	-0.273103
		13	6	0	1.156758	-3.393655	3.629863
		14	6	0	-0.179650	-3.958295	4.123277
		15	6	0	-1.273355	-2.896841	3.978251
		16	6	0	-1.483233	-2.503952	2.508334
		17	6	0	-1.483555	-1.343136	-0.208866
		18	6	0	-2.068619	-2.081699	-1.243431
		19	6	0	-3.291290	-1.650442	-1.778727
		20	6	0	-3.842470	-0.473139	-1.273473
		21	6	0	-3.243045	0.275875	-0.268358
		22	7	0	-2.062056	-0.193330	0.277492
		23	6	0	-1.374841	-3.334410	-1.745823
		24	6	0	-1.984131	-3.890244	-3.040963
		25	6	0	-3.513993	-3.865600	-2.994343
		26	6	0	-4.004475	-2.418751	-2.872922
		27	6	0	-3.831155	1.546656	0.214098
		28	6	0	-3.877909	1.898811	1.574424
		29	6	0	-4.518221	3.068877	1.975672
		30	6	0	-5.107330	3.916075	1.035107
		31	6	0	-5.053080	3.584654	-0.318762
		32	6	0	-4.422021	2.410412	-0.724706
		33	8	0	-1.489099	0.438893	1.250555
		34	14	0	2.017589	3.058237	0.179329
		35	17	0	1.493908	4.943838	0.871179
		36	8	0	0.834826	-1.039980	-1.454704
		37	17	0	2.679619	1.966562	1.817435
		38	17	0	3.631233	3.292117	-1.098046
		39	6	0	0.576061	2.206571	-0.647463

		40	1	0	1.517770	-2.647206	4.352411
		41	1	0	-0.085293	-4.281433	5.165530
		42	1	0	-2.221186	-3.250607	4.397743
		43	1	0	-2.040479	-1.564456	2.455873
		44	1	0	3.153691	-2.847475	1.870418
		45	1	0	-4.794909	-0.121860	-1.656648
		46	1	0	-0.319994	-3.097011	-1.909589
		47	1	0	-1.613231	-4.906982	-3.208575
		48	1	0	-3.939528	-4.328789	-3.890988
		49	1	0	-3.841924	-1.904199	-3.831313
		50	1	0	-2.091813	-3.269044	2.006098
		51	1	0	-0.987072	-2.007746	4.554903
		52	1	0	-0.447151	-4.848008	3.537299
		53	1	0	1.924000	-4.176059	3.595487
		54	1	0	-1.414681	-4.102271	-0.960680
		55	1	0	-1.642223	-3.287375	-3.892313
		56	1	0	-3.867310	-4.451724	-2.135289
		57	1	0	-5.085638	-2.386157	-2.693270
		58	1	0	2.595609	-2.194809	-2.466834
		59	1	0	4.745679	-1.908476	-3.653005
		60	1	0	6.769924	-1.167758	-2.414719
		61	1	0	6.623643	-0.732148	0.031409
		62	1	0	4.482384	-1.039107	1.215679
		63	1	0	-3.401804	1.258677	2.304189
		64	1	0	-4.550953	3.323090	3.031048
		65	1	0	-5.596107	4.831805	1.354518
		66	1	0	-5.492875	4.243166	-1.061917
		67	1	0	-4.362317	2.172121	-1.782175
		68	1	0	-0.114247	1.907470	0.156017
		69	6	0	-0.115258	3.062414	-1.673558
		70	1	0	0.953826	1.276513	-1.093259
		71	6	0	-0.047848	2.867285	-2.991888
		72	1	0	-0.706663	3.892002	-1.288058
		73	1	0	-0.570430	3.518057	-3.686677
		74	1	0	0.524346	2.047578	-3.418190

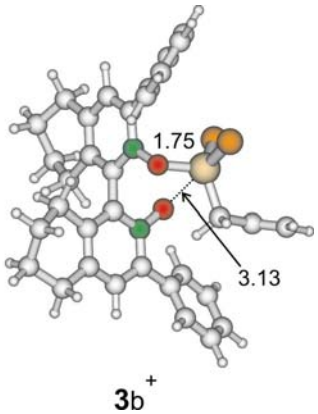
Three most stable arrangements found for the complex [1•$SiCl_2(C_3H_5)$]$^+$



$\mathbf{3}^+$



$\mathbf{3a}^+$



$\mathbf{3b}^+$

Note that the considered isomer $\mathbf{3}^+$ is the most stable form in all solvents.

Isomer	Total energy/Hartree ZPE/Hartree PCM energy/Hartree	Geometry Center Number / Atomic Number / Atomic Type / Coordinates (Angstroms) X Y Z
3^{+}	E_{tot}: -2747.1220737 ZPE: 0.592579 ACN: -2747.192199 DCM: -2747.184117 PhCl: -2747.177566 TOL: -2747.158998	1 6 0 -2.476908 3.573501 2.783809 2 6 0 -2.104606 2.567581 1.715311 3 6 0 -0.789548 2.468479 1.203756 4 6 0 0.315257 3.379025 1.714513 5 6 0 -0.025490 4.028890 3.062597 6 6 0 -1.419450 4.658009 3.013256 7 6 0 -3.076791 1.700319 1.226636 8 6 0 -2.803473 0.699607 0.293167 9 7 0 -1.509278 0.615778 -0.134666 10 6 0 -0.531557 1.489036 0.242015 11 6 0 0.824630 1.301570 -0.345484 12 6 0 1.439992 2.197464 -1.214066 13 6 0 2.808066 1.985084 -1.507488 14 6 0 3.472150 0.945809 -0.861531 15 6 0 2.823997 0.017826 -0.040988 16 7 0 1.481247 0.198060 0.122668 17 6 0 0.667724 3.348901 -1.834179 18 6 0 1.344560 3.894140 -3.100089 19 6 0 2.828428 4.164946 -2.836828 20 6 0 3.555123 2.859697 -2.491508 21 8 0 0.717794 -0.735095 0.723257 22 14 0 -0.413877 -1.911373 -0.492720 23 6 0 -0.896276 -2.771787 1.131746 24 6 0 -0.510866 -4.228300 1.125336 25 6 0 0.446738 -4.754396 1.890462 26 8 0 -1.179156 -0.361788 -1.028917 27 17 0 -1.747836 -2.983144 -1.800073 28 17 0 1.305312 -2.317126 -1.620255 29 1 0 3.694304 2.269105 -3.408191 30 1 0 3.300600 4.623992 -3.710002 31 1 0 0.831086 4.807500 -3.414321 32 1 0 -0.356442 3.030600 -2.053212 33 6 0 3.541965 -1.071026 0.645993 34 1 0 4.540730 0.825300 -0.999044 35 6 0 -3.860467 -0.197470 -0.208755 36 1 0 -4.103104 1.794712 1.562299 37 1 0 1.252286 2.818995 1.785885 38 1 0 0.734483 4.779635 3.297514 39 1 0 -1.641397 5.191852 3.941463 40 1 0 -2.632661 3.011992 3.715984 41 1 0 0.587938 4.165499 -1.104743 42 1 0 1.237416 3.172161 -3.919134 43 1 0 2.930994 4.880915 -2.011126 44 1 0 4.562201 3.056361 -2.107748 45 1 0 0.489800 4.175287 0.979988

		46	1	0	0.014700	3.276967	3.860774
		47	1	0	-1.461275	5.399644	2.205562
		48	1	0	-3.449811	4.012216	2.535755
		49	1	0	-0.442082	-2.255333	1.979383
		50	1	0	-1.987891	-2.672934	1.200102
		51	1	0	-1.059336	-4.865027	0.435338
		52	1	0	0.686020	-5.811967	1.846375
		53	1	0	1.023422	-4.150291	2.586301
		54	6	0	3.251805	-1.411979	1.978443
		55	6	0	4.015824	-2.372735	2.634551
		56	6	0	5.062257	-3.016283	1.970041
		57	6	0	5.349192	-2.690673	0.643474
		58	6	0	4.599684	-1.719415	-0.014001
		59	1	0	2.437337	-0.921021	2.496690
		60	1	0	3.794508	-2.619449	3.668101
		61	1	0	5.649230	-3.771329	2.483286
		62	1	0	6.152329	-3.196847	0.118016
		63	1	0	4.812789	-1.489872	-1.053139
		64	6	0	-4.036293	-0.443786	-1.580980
		65	6	0	-5.121919	-1.197797	-2.015130
		66	6	0	-6.024888	-1.731747	-1.093969
		67	6	0	-5.848937	-1.502764	0.272234
		68	6	0	-4.780044	-0.729258	0.714625
		69	1	0	-3.331354	-0.047866	-2.300955
		70	1	0	-5.255496	-1.378290	-3.076408
		71	1	0	-6.861956	-2.329809	-1.439775
		72	1	0	-6.541971	-1.925653	0.992038
		73	1	0	-4.642360	-0.557819	1.778053
3a^{+}	E_{tot}: -2747.1243018 ZPE: 0.591785 ACN: -2747.186384 DCM: -2747.179121 PhCl: -2747.173339 TOL: -2747.156959	1	6	0	4.818130	-0.496360	-1.000529
		2	6	0	3.864973	-0.083506	-0.053530
		3	6	0	4.091934	-0.334836	1.310618
		4	6	0	5.255193	-0.984388	1.713597
		5	6	0	6.193703	-1.400285	0.766976
		6	6	0	5.971440	-1.159032	-0.590140
		7	6	0	2.709881	0.717462	-0.505967
		8	6	0	2.856968	1.790330	-1.378714
		9	6	0	1.789313	2.601647	-1.765637
		10	6	0	0.521062	2.368233	-1.195375
		11	6	0	0.373616	1.306124	-0.301705
		12	7	0	1.438915	0.486955	-0.052255
		13	6	0	-0.676970	3.240967	-1.519198
		14	6	0	-0.456013	4.138594	-2.745746
		15	6	0	0.924242	4.798632	-2.708897
		16	6	0	2.018194	3.725511	-2.749549
		17	8	0	1.207045	-0.603877	0.757006
		18	14	0	0.930733	-2.211322	0.125998
		19	6	0	-0.855375	-2.723744	0.283518
		20	6	0	-0.878448	1.096602	0.481610
		21	6	0	-1.068830	1.608318	1.764932
		22	6	0	-2.337431	1.445431	2.353293

		23	6	0	-3.317013	0.780388	1.616290
		24	6	0	-3.104243	0.249055	0.343629
		25	7	0	-1.853650	0.428771	-0.210388
		26	6	0	-2.647494	1.969076	3.740916
		27	6	0	-1.645036	3.024297	4.222226
		28	6	0	-0.212328	2.545022	3.972960
		29	6	0	0.048412	2.356990	2.471366
		30	6	0	-4.150524	-0.491526	-0.392140
		31	6	0	-4.328674	-0.374125	-1.782819
		32	6	0	-5.381429	-1.034139	-2.411686
		33	6	0	-6.259940	-1.832027	-1.676513
		34	6	0	-6.083362	-1.967365	-0.298763
		35	6	0	-5.040418	-1.300868	0.338552
		36	8	0	-1.538261	-0.033998	-1.383205
		37	17	0	1.592181	-2.252366	-1.816242
		38	17	0	2.129062	-3.354180	1.342121
		39	1	0	-2.641211	1.120217	4.439597
		40	1	0	-1.805257	3.226347	5.285350
		41	1	0	0.514135	3.256057	4.377958
		42	1	0	1.000545	1.836844	2.321572
		43	1	0	-4.311917	0.675139	2.034924
		44	1	0	3.857676	2.003882	-1.736237
		45	1	0	-1.542249	2.592931	-1.682963
		46	1	0	-1.248162	4.891872	-2.783274
		47	1	0	1.052366	5.481075	-3.553827
		48	1	0	2.053283	3.278492	-3.753784
		49	1	0	0.161672	3.343349	1.998985
		50	1	0	-0.049437	1.594028	4.495991
		51	1	0	-1.815434	3.970356	3.691962
		52	1	0	-3.669125	2.364194	3.758168
		53	1	0	-0.905820	3.862500	-0.642860
		54	1	0	-0.548996	3.538826	-3.659672
		55	1	0	1.027000	5.400783	-1.797101
		56	1	0	3.010433	4.157152	-2.578871
		57	1	0	-3.641415	0.226861	-2.362180
		58	1	0	-5.513296	-0.926643	-3.483801
		59	1	0	-7.073128	-2.350282	-2.175046
		60	1	0	-6.752664	-2.596167	0.279686
		61	1	0	-4.901422	-1.430328	1.407493
		62	1	0	3.369232	-0.013960	2.052098
		63	1	0	5.428529	-1.166247	2.769150
		64	1	0	7.095451	-1.912802	1.086407
		65	1	0	6.693782	-1.488928	-1.329444
		66	1	0	4.640700	-0.322335	-2.057037
		67	6	0	-1.026419	-4.207939	0.072550
		68	1	0	-1.201157	-2.418233	1.279849
		69	1	0	-1.406930	-2.146094	-0.466861
		70	6	0	-1.535216	-4.750343	-1.034543
		71	1	0	-0.695393	-4.851759	0.884863
		72	1	0	-1.633340	-5.825922	-1.139426

		73	1	0	-1.878363	-4.141678	-1.866957
3b$^+$	E_{tot}: -2747.1217365 ZPE: 0.591898 ACN: -2747.18371 DCM: -2747.176269 PhCl: -2747.170431 TOL: -2747.154475	1	6	0	4.762129	-0.814500	-0.693439
		2	6	0	3.821529	-0.233365	0.172882
		3	6	0	3.992972	-0.347189	1.563109
		4	6	0	5.093000	-1.029844	2.072567
		5	6	0	6.018862	-1.616877	1.206942
		6	6	0	5.849687	-1.512532	-0.174767
		7	6	0	2.739215	0.597368	-0.390175
		8	6	0	2.988539	1.598866	-1.322994
		9	6	0	1.988726	2.440820	-1.810284
		10	6	0	0.687472	2.321692	-1.277111
		11	6	0	0.440921	1.329355	-0.327433
		12	7	0	1.441394	0.466315	0.018981
		13	6	0	-0.440481	3.238609	-1.716702
		14	6	0	-0.129333	3.986725	-3.020734
		15	6	0	1.278836	4.585175	-2.986277
		16	6	0	2.322107	3.468667	-2.867564
		17	8	0	1.097882	-0.575318	0.850840
		18	14	0	0.799424	-2.192873	0.240830
		19	6	0	-0.900567	-2.792917	0.751910
		20	6	0	-0.866216	1.235905	0.385151
		21	6	0	-1.191588	2.008446	1.498150
		22	6	0	-2.505770	1.915007	1.997120
		23	6	0	-3.394331	1.065426	1.339264
		24	6	0	-3.043261	0.271616	0.245905
		25	7	0	-1.745764	0.372035	-0.209936
		26	6	0	-2.956521	2.700590	3.211688
		27	6	0	-2.023029	3.867151	3.556760
		28	6	0	-0.563581	3.403736	3.531308
		29	6	0	-0.165388	2.937871	2.123259
		30	6	0	-3.994243	-0.653713	-0.404974
		31	6	0	-4.023200	-0.847532	-1.798276
		32	6	0	-4.991763	-1.668738	-2.369976
		33	6	0	-5.931939	-2.320727	-1.569491
		34	6	0	-5.902825	-2.146217	-0.185290
		35	6	0	-4.944563	-1.317475	0.392483
		36	8	0	-1.287996	-0.350022	-1.189278
		37	17	0	1.259851	-2.223616	-1.759373
		38	17	0	2.187231	-3.358494	1.228469
		39	1	0	-3.003602	2.011563	4.066975
		40	1	0	-2.284204	4.268222	4.540406
		41	1	0	0.107540	4.207966	3.847744
		42	1	0	0.814380	2.448519	2.151431
		43	1	0	-4.423333	1.012197	1.677874
		44	1	0	4.014226	1.725274	-1.650266
		45	1	0	-1.355770	2.650443	-1.828653
		46	1	0	-0.881011	4.766766	-3.172278
		47	1	0	1.475455	5.171214	-3.888407
		48	1	0	2.396508	2.934779	-3.826118
		49	1	0	-0.046403	3.818494	1.476029

		50	1	0	-0.428483	2.580169	4.243938
		51	1	0	-2.162644	4.683372	2.836012
		52	1	0	-3.981572	3.053896	3.054523
		53	1	0	-0.636045	3.966302	-0.917550
		54	1	0	-0.214829	3.297545	-3.870087
		55	1	0	1.370172	5.273718	-2.136501
		56	1	0	3.321391	3.873427	-2.673317
		57	1	0	-3.286632	-0.359207	-2.421957
		58	1	0	-5.010025	-1.801634	-3.447172
		59	1	0	-6.678895	-2.965857	-2.021393
		60	1	0	-6.621244	-2.659106	0.446151
		61	1	0	-4.919579	-1.204572	1.472043
		62	1	0	3.275556	0.104636	2.239307
		63	1	0	5.227013	-1.105687	3.146638
		64	1	0	6.870822	-2.155508	1.609386
		65	1	0	6.562996	-1.974834	-0.849039
		66	1	0	4.625278	-0.742135	-1.767793
		67	6	0	-1.425225	-3.826835	-0.213115
		68	1	0	-0.783832	-3.216433	1.755583
		69	1	0	-1.579527	-1.941065	0.815845
		70	6	0	-1.452907	-5.137977	0.028281
		71	1	0	-1.788497	-3.434964	-1.160079
		72	1	0	-1.841514	-5.836562	-0.705513
		73	1	0	-1.098125	-5.560095	0.965106

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