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SUPPLEMENTARY MATERIAL TO

Mechanistic, energetic and structural studies of single-walled carbon nanotubes functionalized with penicillamine

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CARTESIAN COORDINATES, SUM OF ELECTRONIC AND ZERO-POINT ENERGIES (*E*), SUM OF ELECTRONIC AND THERMAL ENTHALPIES (*H*) AND GIBBS ENERGIES (*G*) FOR THE CALCULATED STRUCTURES

In water

NTCOOH

C	–4.899397	–2.146763	–2.963260
C	–4.899166	–3.159030	–2.035517
C	–3.701830	–3.494569	–1.325958
C	–3.702526	–3.765140	0.098873
C	–2.476948	–3.627792	0.803484
C	–2.477128	–2.991279	2.090512
C	–1.230843	–2.488745	2.593937
C	–1.229466	–1.221036	3.237048
C	0.000006	–0.519475	3.365658
C	–0.000004	0.898416	3.135210
C	1.223742	1.539153	2.814654
C	1.217941	2.599525	1.865479
C	2.485670	3.009147	1.295816
C	2.501168	3.306701	–0.121748
C	3.730174	3.187182	–0.823237
C	3.717802	2.529042	–2.105523
C	4.912255	2.021834	–2.720980
C	4.903886	0.804858	–3.350516
C	–4.899296	–3.711905	0.879486
C	–4.898040	–3.101484	2.111953
C	–3.701864	–2.519002	2.631367

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(CC) 2018 SCS.

C	–3.700494	–1.221244	3.290362
C	–2.471666	–0.511777	3.354440
C	–2.468250	0.906911	3.146812
C	–1.223757	1.539137	2.814653
C	–1.217971	2.599508	1.865478
C	–0.000017	2.995770	1.286633
C	–0.000020	3.656055	–0.097954
C	1.270296	3.230081	–0.831771
C	1.245788	2.510334	–2.026632
C	2.484381	1.996171	–2.555492
C	2.477073	0.724238	–3.220878
C	3.701670	0.025941	–3.411470
C	3.700996	–1.408149	–3.231191
C	4.899435	–2.146697	–2.963257
C	4.899217	–3.158965	–2.035514
C	–4.888960	–0.458031	3.474312
C	–4.882382	0.909828	3.291018
C	–3.689025	1.588159	2.913349
C	–3.688632	2.679330	1.941361
C	–2.485704	3.009113	1.295814
C	–2.501205	3.306667	–0.121750
C	–1.270331	3.230063	–0.831772
C	–1.245813	2.510318	–2.026633
C	–0.000009	2.000709	–2.543015
C	0.000000	0.742457	–3.175533
C	1.235482	0.025977	–3.325768
C	1.233238	–1.380793	–3.168892
C	2.475149	–2.040505	–2.892150
C	2.475281	–3.103411	–1.925460
C	3.701885	–3.494520	–1.325956
C	3.702584	–3.765090	0.098875
C	4.899353	–3.711838	0.879489
C	4.898088	–3.101417	2.111956
C	–4.909600	3.093561	1.300156
C	–4.931161	3.326640	–0.047879
C	–3.730209	3.187133	–0.823240
C	–3.717828	2.528992	–2.105526
C	–2.484398	1.996138	–2.555495
C	–2.477073	0.724205	–3.220880
C	–1.235473	0.025960	–3.325769
C	–1.233210	–1.380809	–3.168893
C	0.000018	–2.043028	–2.883300
C	0.000025	–3.096650	–1.926869
C	1.233262	–3.446715	–1.298424
C	1.231975	–3.718328	0.095465
C	2.477004	–3.627759	0.803485
C	2.477174	–2.991245	2.090513

(CC) 2018 SCS.

C	3.701903	–2.518951	2.631369
C	3.700515	–1.221194	3.290364
C	4.888971	–0.457965	3.474315
C	4.882375	0.909894	3.291022
C	–4.912272	2.021768	–2.720984
C	–4.903887	0.804792	–3.350520
C	–3.701661	0.025892	–3.411472
C	–3.700967	–1.408199	–3.231193
C	–2.475113	–2.040538	–2.892152
C	–2.475231	–3.103444	–1.925461
C	–1.233208	–3.446731	–1.298425
C	–1.231917	–3.718345	0.095464
C	0.000028	–3.638324	0.808584
C	0.000023	–3.001603	2.092374
C	1.230883	–2.488728	2.593938
C	1.229488	–1.221019	3.237049
C	2.471678	–0.511743	3.354442
C	2.468243	0.906945	3.146815
C	3.689009	1.588209	2.913352
C	3.688602	2.679381	1.941364
C	4.909565	3.093628	1.300160
C	4.931124	3.326706	–0.047875
H	–5.883959	3.482254	–0.542682
H	–5.845021	3.077940	1.848607
H	–5.831150	1.435294	3.292029
H	–5.842218	–0.958489	3.606105
H	–5.846665	–2.932183	2.610281
H	–5.847791	–4.005204	0.442516
H	–5.846336	–3.598386	–1.741249
H	–5.845753	–1.816509	–3.377808
H	–5.844169	0.378695	–3.683872
H	–5.857450	2.532289	–2.570510
H	5.844174	0.378773	–3.683868
H	5.857425	2.532367	–2.570506
H	5.883920	3.482332	–0.542678
H	5.844985	3.078019	1.848612
H	5.831136	1.435373	3.292034
H	5.842236	–0.958410	3.606109
H	5.846710	–2.932103	2.610285
H	5.847852	–4.005125	0.442520
H	5.846393	–3.598307	–1.741246
H	5.845787	–1.816431	–3.377804
C	–0.000032	5.211032	–0.062834
O	–0.000119	5.899911	–1.061235
O	–0.000187	5.712920	1.182516
H	–0.000297	6.684006	1.103421

E = –3630.141426, H = –3630.094310, G = –3630.206697 a.u.

(CC) 2018 SCS.

PCA

C	–0.414380	0.596098	–0.596400
C	–1.590579	–0.141967	0.042263
C	0.965825	0.210924	0.048526
O	–2.175354	–1.011821	–0.800087
N	–0.770427	2.015424	–0.553214
S	1.155922	–1.654534	0.028771
O	–1.997558	0.061330	1.169933
C	1.074388	0.617047	1.526058
C	2.104483	0.846269	–0.762275
H	–0.371385	0.299192	–1.648553
H	–2.920630	–1.421038	–0.324234
H	–0.064411	2.578750	–1.017816
H	–0.835667	2.331235	0.410890
H	1.118880	–1.821718	–1.309144
H	2.053228	0.335317	1.923781
H	0.295825	0.155896	2.135859
H	0.981901	1.703620	1.618707
H	3.074121	0.547690	–0.356833
H	2.046585	1.939310	–0.713273
H	2.064669	0.550032	–1.815014

E = –800.417185, H = –800.405236, G = –800.453188 a.u.

NTCOOH/PCA1R

C	–4.192949	–4.208062	3.142135
C	–5.242459	–3.953744	2.293787
C	–5.332753	–2.702903	1.603367
C	–5.702814	–2.621965	0.203142
C	–5.328429	–1.457335	–0.518062
C	–4.809786	–1.595658	–1.849824
C	–4.062034	–0.500794	–2.398878
C	–2.883413	–0.796980	–3.136209
C	–1.918769	0.229201	–3.327055
C	–0.529055	–0.114177	–3.206288
C	0.408780	0.916231	–2.942247
C	1.506177	0.643903	–2.078685
C	2.248833	1.769928	–1.549570
C	2.651647	1.694503	–0.160951
C	2.889099	2.906597	0.540563
C	2.345512	3.038508	1.869696
C	2.188682	4.312652	2.513425
C	1.055515	4.590993	3.232058
C	–5.999867	–3.786483	–0.571353
C	–5.502721	–3.917716	–1.847134
C	–4.688830	–2.891588	–2.416832
C	–3.482014	–3.194848	–3.172260
C	–2.504727	–2.171834	–3.298281

(CC) 2018 SCS.

C	–1.115176	–2.511492	–3.200729
C	–0.178221	–1.459372	–2.927966
C	0.923699	–1.720264	–2.064734
C	1.643494	–0.640864	–1.524209
C	2.384555	–0.819695	–0.193448
C	2.332409	0.509212	0.559354
C	1.723518	0.645182	1.807941
C	1.565147	1.965029	2.365981
C	0.382417	2.257115	3.125033
C	0.016181	3.611730	3.359331
C	–1.385398	3.958296	3.288762
C	–1.832515	5.302171	3.070983
C	–2.883404	5.556282	2.224326
C	–3.043091	–4.529428	–3.406153
C	–1.703769	–4.853643	–3.329106
C	–0.731530	–3.863047	–3.013382
C	0.398986	–4.136943	–2.128083
C	1.056102	–3.056203	–1.517293
C	1.444309	–3.159078	–0.125846
C	1.722248	–1.953885	0.577879
C	1.121251	–1.772997	1.823370
C	0.967705	–0.446849	2.368416
C	–0.200560	–0.150972	3.096427
C	–0.584499	1.218958	3.291482
C	–1.957978	1.557063	3.242158
C	–2.318206	2.924555	3.008540
C	–3.421040	3.191671	2.127180
C	–3.550203	4.483218	1.550995
C	–3.920579	4.565469	0.151111
C	–3.642233	5.723212	–0.640194
C	–3.147019	5.589865	–1.916439
C	0.552425	–5.428850	–1.511225
C	0.873489	–5.521545	–0.184390
C	1.086532	–4.331686	0.590684
C	0.550096	–4.177092	1.919920
C	0.365979	–2.857180	2.400120
C	–0.811911	–2.551477	3.161133
C	–1.180082	–1.179311	3.309671
C	–2.552319	–0.836843	3.260257
C	–2.917658	0.522815	3.017930
C	–4.010533	0.787498	2.145822
C	–4.100339	2.075905	1.537526
C	–4.469079	2.155948	0.168548
C	–4.136668	3.351103	–0.552945
C	–3.618572	3.213193	–1.884983
C	–2.909367	4.294905	–2.469970
C	–1.703067	3.989228	–3.225349

(CC) 2018 SCS.

C	–0.692562	4.961659	–3.473804
C	0.643355	4.624691	–3.393604
C	–0.181082	–5.221328	2.581372
C	–1.308528	–4.927558	3.302602
C	–1.767816	–3.574025	3.414332
C	–3.169150	–3.225999	3.343551
C	–3.511030	–1.880381	3.044474
C	–4.612947	–1.613537	2.162094
C	–4.693993	–0.317909	1.554902
C	–5.061876	–0.235348	0.185891
C	–4.743547	0.949573	–0.539764
C	–4.224723	0.811334	–1.868656
C	–3.470287	1.888349	–2.416465
C	–2.292486	1.589625	–3.153953
C	–1.316677	2.626809	–3.333633
C	0.070903	2.280412	–3.233433
C	1.040949	3.299166	–3.060241
C	2.170952	3.024356	–2.175046
C	2.917279	4.100786	–1.576637
C	3.254833	4.048151	–0.251747
H	0.829325	–6.488921	0.304707
H	0.268482	–6.326352	–2.049738
H	–1.423379	–5.900776	–3.363574
H	–3.766274	–5.333255	–3.491922
H	–5.606007	–4.873044	–2.350766
H	–6.479700	–4.641368	–0.107180
H	–5.917947	–4.763865	2.040155
H	–4.070063	–5.210699	3.537202
H	–1.922070	–5.741323	3.674294
H	0.073883	–6.259863	2.399170
H	0.895076	5.602549	3.589481
H	2.899411	5.108716	2.318679
H	3.673844	4.928821	0.223339
H	3.085236	5.019245	–2.128349
H	1.380054	5.419358	–3.439504
H	–0.957765	6.008771	–3.572883
H	–2.794204	6.475901	–2.433482
H	–3.664611	6.709385	–0.189095
H	–3.103433	6.584712	1.958237
H	–1.253345	6.136420	3.451959
C	3.903080	–1.151856	–0.349322
O	4.554895	–1.598492	0.583264
O	4.392310	–0.850235	–1.536022
H	5.417564	–0.963822	–1.527646
C	7.666899	–0.928858	–0.226874
C	7.095230	0.272524	0.526555
C	9.240343	–0.920688	–0.228971

(CC) 2018 SCS.

O	6.568754	1.201431	–0.291428
N	7.061347	–1.024984	–1.564969
S	9.786475	–1.049438	1.569328
O	7.135233	0.395481	1.732765
C	9.810097	0.361289	–0.854491
C	9.755658	–2.160875	–0.976969
H	7.336558	–1.804133	0.337661
H	6.230736	1.927562	0.262366
H	7.342575	–1.891870	–2.015702
H	7.361228	–0.258453	–2.164112
H	11.031387	–1.480170	1.283545
H	10.902575	0.328723	–0.853984
H	9.499219	1.255783	–0.309267
H	9.487652	0.462172	–1.897546
H	10.844796	–2.222116	–0.904848
H	9.511769	–2.102860	–2.042685
H	9.332718	–3.082976	–0.568442

E = –4430.574241, H = –4430.513781, G = –4430.658880 a.u.

TS_{k1}

C	5.058597	–3.420958	–2.807358
C	5.923540	–3.051702	–1.806686
C	5.713305	–1.840229	–1.073430
C	5.867707	–1.776080	0.367338
C	5.213055	–0.723748	1.061023
C	4.544157	–1.011570	2.298453
C	3.557038	–0.079197	2.762808
C	2.349565	–0.596642	3.305079
C	1.212093	0.251826	3.380007
C	–0.071363	–0.298850	3.043389
C	–1.121746	0.581138	2.683156
C	–2.034771	0.183607	1.664700
C	–2.859630	1.217723	1.068444
C	–3.026744	1.164864	–0.369373
C	–3.351983	2.365244	–1.055795
C	–2.667988	2.644720	–2.290689
C	–2.635113	3.957218	–2.873433
C	–1.474460	4.443950	–3.414273
C	6.238804	–2.919416	1.141413
C	5.597725	–3.193534	2.327026
C	4.557452	–2.338379	2.803003
C	3.322033	–2.867239	3.362692
C	2.181928	–2.020094	3.367972
C	0.895661	–2.568282	3.053033
C	–0.154033	–1.664922	2.671382
C	–1.070962	–2.051551	1.654934
C	–1.898949	–1.078999	1.056793

(CC) 2018 SCS.

C	–2.405954	–1.293086	–0.382576
C	–2.443727	0.072136	–1.071333
C	–1.692546	0.371536	–2.212449
C	–1.668211	1.728524	–2.700969
C	–0.455409	2.240321	–3.272882
C	–0.283426	3.645815	–3.413642
C	1.018336	4.202853	–3.125654
C	1.205039	5.586787	–2.803372
C	2.067094	5.956076	–1.800379
C	3.079432	–4.264781	3.490226
C	1.836716	–4.791336	3.202339
C	0.771889	–3.950760	2.770743
C	–0.159028	–4.349781	1.718320
C	–0.892498	–3.356258	1.053093
C	–1.067896	–3.442325	–0.378355
C	–1.446947	–2.259652	–1.074360
C	–0.713775	–1.918128	–2.212526
C	–0.700640	–0.557554	–2.689573
C	0.496805	–0.044507	–3.227117
C	0.679361	1.375974	–3.324401
C	1.959365	1.921617	–3.063813
C	2.056651	3.314108	–2.739093
C	2.963661	3.702993	–1.695176
C	2.796932	4.966087	–1.067614
C	2.946004	5.029735	0.373597
C	2.371666	6.084611	1.149367
C	1.729294	5.806110	2.333344
C	–0.010945	–5.615129	1.046075
C	–0.131105	–5.685543	–0.314291
C	–0.429969	–4.502379	–1.073191
C	0.249079	–4.194825	–2.306367
C	0.281717	–2.837345	–2.708326
C	1.490825	–2.311759	–3.275377
C	1.650098	–0.893718	–3.324392
C	2.928413	–0.345010	–3.063950
C	3.031975	1.039919	–2.730206
C	3.932991	1.425376	–1.698408
C	3.725741	2.677847	–1.045449
C	3.880585	2.741750	0.364779
C	3.257741	3.828785	1.064931
C	2.586896	3.539668	2.301059
C	1.633756	4.462163	2.807360
C	0.401330	3.929230	3.369235
C	–0.778384	4.715112	3.507828
C	–2.017849	4.177135	3.227745
C	1.224083	–5.074405	–2.888622
C	2.380243	–4.569784	–3.423376

(CC) 2018 SCS.

C	2.626121	–3.157410	–3.418113
C	3.928185	–2.600650	–3.128147
C	4.003141	–1.236204	–2.740957
C	4.912155	–0.848178	–1.698463
C	4.697067	0.410361	–1.047314
C	4.852208	0.477044	0.362617
C	4.246673	1.557447	1.068880
C	3.575688	1.268521	2.301870
C	2.585103	2.181641	2.764297
C	1.379180	1.660858	3.307639
C	0.231535	2.518809	3.374786
C	–1.053290	1.963789	3.064681
C	–2.144144	2.827127	2.793903
C	–3.075685	2.433281	1.740768
C	–3.884599	3.416897	1.070191
C	–4.004399	3.390304	–0.292688
H	0.134269	–6.605949	–0.823607
H	0.338512	–6.484429	1.592317
H	1.728941	–5.869895	3.164341
H	3.904974	–4.947307	3.661659
H	5.782359	–4.146829	2.810706
H	6.909023	–3.664146	0.725732
H	6.678857	–3.759241	–1.481354
H	5.155737	–4.408232	–3.245953
H	3.163186	–5.256117	–3.728049
H	1.115955	–6.148556	–2.782292
H	–1.431472	5.483969	–3.719839
H	–3.486187	4.620396	–2.761938
H	–4.480572	4.223881	–0.797848
H	–4.272774	4.267892	1.618777
H	–2.874775	4.841190	3.198745
H	–0.703779	5.783012	3.682536
H	1.164683	6.595676	2.817831
H	2.294426	7.084444	0.735989
H	2.076149	6.990321	–1.473097
H	0.558410	6.339257	–3.241768
C	–3.851124	–1.929697	–0.552034
O	–4.234105	–2.362616	–1.627685
O	–3.817435	–3.222485	0.815507
H	–4.271100	–3.975912	0.407451
C	–6.333062	–1.455184	–0.115260
C	–6.556360	–0.766403	–1.462777
C	–7.370704	–1.036670	0.983278
O	–5.912121	0.407114	–1.551060
N	–4.952316	–1.293500	0.390301
S	–9.059405	–1.423259	0.245729
O	–7.278338	–1.209449	–2.329651

(CC) 2018 SCS.

C	–7.297882	0.455646	1.342802
C	–7.171093	–1.904507	2.236994
H	–6.465461	–2.519544	–0.314604
H	–6.101800	0.795802	–2.423354
H	–4.654722	–2.198522	1.069240
H	–4.733474	–0.341597	0.686137
H	–9.729227	–1.246254	1.401002
H	–8.065332	0.694362	2.083544
H	–7.450025	1.096591	0.472926
H	–6.330612	0.706918	1.793439
H	–7.957542	–1.696120	2.966947
H	–6.214830	–1.678036	2.718901
H	–7.199364	–2.970414	1.996623

E = –4430.490813, H = –4430.431051, G = –4430.571473 a.u.

NTCON/H_2OP

C	–3.818651	–4.661648	2.706953
C	–4.758171	–4.545422	1.712218
C	–4.924498	–3.309229	1.009686
C	–5.095538	–3.259894	–0.429688
C	–4.789671	–2.043143	–1.095249
C	–4.068867	–2.086740	–2.336206
C	–3.410670	–0.889757	–2.775286
C	–2.106523	–1.006337	–3.328191
C	–1.278917	0.148051	–3.379915
C	0.110812	0.001448	–3.050015
C	0.847617	1.150051	–2.663095
C	1.836328	1.023494	–1.647540
C	2.328392	2.234390	–1.022797
C	2.525605	2.196732	0.412297
C	2.479163	3.420826	1.131270
C	1.735639	3.454835	2.365434
C	1.308464	4.683978	2.973414
C	0.055393	4.788165	3.517878
C	–5.109558	–4.442883	–1.232882
C	–4.418522	–4.483280	–2.421193
C	–3.684225	–3.344035	–2.871523
C	–2.349598	–3.463339	–3.439066
C	–1.518374	–2.311670	–3.424924
C	–0.125086	–2.455099	–3.120126
C	0.603352	–1.286452	–2.717712
C	1.592168	–1.403633	–1.701109
C	2.072405	–0.239411	–1.070246
C	2.630103	–0.327074	0.359729
C	2.277813	0.968010	1.086219
C	1.477530	0.998682	2.228622
C	1.052230	2.274287	2.748265

(CC) 2018 SCS.

C	–0.256987	2.384534	3.325658
C	–0.841851	3.670019	3.496509
C	–2.252668	3.816323	3.218612
C	–2.848908	5.086970	2.929647
C	–3.788738	5.203147	1.935271
C	–1.697387	–4.719734	–3.599000
C	–0.352555	–4.854510	–3.320832
C	0.412894	–3.742172	–2.869657
C	1.427580	–3.867588	–1.825903
C	1.830851	–2.714401	–1.132528
C	2.027072	–2.780012	0.300875
C	2.024902	–1.557861	1.029906
C	1.230772	–1.480333	2.174412
C	0.811656	–0.197345	2.680563
C	–0.481189	–0.080706	3.226294
C	–1.080413	1.217925	3.354412
C	–2.465760	1.359479	3.101916
C	–2.978164	2.665676	2.809996
C	–3.966469	2.787849	1.774320
C	–4.190995	4.056872	1.177806
C	–4.359937	4.107074	–0.261745
C	–4.134562	5.304594	–1.009690
C	–3.443176	5.261708	–2.197932
C	1.672378	–5.133526	–1.185468
C	1.808712	–5.198125	0.174414
C	1.737558	–4.001267	0.965160
C	0.998435	–3.942654	2.201186
C	0.560606	–2.668653	2.640222
C	–0.747900	–2.543747	3.217122
C	–1.325259	–1.240061	3.299605
C	–2.710066	–1.094216	3.046217
C	–3.225272	0.203599	2.744587
C	–4.205042	0.324496	1.719686
C	–4.387229	1.596643	1.097708
C	–4.559582	1.644589	–0.311057
C	–4.297166	2.885179	–0.982925
C	–3.575912	2.841928	–2.223702
C	–2.947838	4.021145	–2.703871
C	–1.613187	3.898812	–3.272042
C	–0.724542	5.007067	–3.378594
C	0.619389	4.860309	–3.102116
C	0.334637	–5.089071	2.756116
C	–0.917134	–4.967902	3.299988
C	–1.575796	–3.694789	3.332007
C	–2.986244	–3.547490	3.051857
C	–3.468366	–2.259264	2.697569
C	–4.456405	–2.137553	1.661660

(CC) 2018 SCS.

C	–4.631576	–0.857401	1.041750
C	–4.804258	–0.806770	–0.366859
C	–4.554186	0.422224	–1.044786
C	–3.832051	0.378555	–2.281737
C	–3.165673	1.559307	–2.719372
C	–1.861872	1.439948	–3.272552
C	–1.026514	2.605936	–3.313466
C	0.366671	2.456676	–3.009865
C	1.147770	3.599295	–2.704845
C	2.163323	3.474736	–1.662084
C	2.650835	4.637536	–0.966699
C	2.789945	4.613701	0.394120
H	1.831816	–6.168917	0.658178
H	1.599024	–6.054325	–1.753460
H	0.074856	–5.851213	–3.308412
H	–2.279724	–5.614975	–3.788579
H	–4.311150	–5.435533	–2.929610
H	–5.526217	–5.363700	–0.839204
H	–5.266649	–5.439036	1.366284
H	–3.612678	–5.642894	3.120716
H	–1.456542	–5.865391	3.583369
H	0.758982	–6.078223	2.621606
H	–0.296849	5.760771	3.844609
H	1.920326	5.574920	2.881332
H	3.003415	5.538058	0.920210
H	2.765366	5.578643	–1.493188
H	1.235695	5.750975	–3.047160
H	–1.117733	6.007345	–3.524499
H	–3.145627	6.196265	–2.661552
H	–4.360793	6.270596	–0.571282
H	–4.110924	6.194075	1.633434
H	–2.456255	5.988564	3.387233
C	4.186545	–0.489662	0.453633
O	4.734511	–0.553167	1.555109
O	6.954004	–0.235448	3.417746
H	7.525079	–0.775685	2.852417
C	6.298925	–0.763486	–0.842128
C	6.807835	–1.742926	0.225010
C	7.088863	0.579967	–0.946575
O	6.103505	–2.882276	0.207068
N	4.854743	–0.570465	–0.717208
S	8.899039	0.119092	–1.213550
O	7.779003	–1.571381	0.936702
C	6.954621	1.470955	0.295997
C	6.593196	1.338731	–2.188757
H	6.447530	–1.292609	–1.790009
H	6.481684	–3.474199	0.881085

(CC) 2018 SCS.

H	4.309892	–0.541863	–1.568799
H	6.121062	–0.254691	2.918778
H	9.097681	0.916020	–2.281234
H	7.544775	2.380448	0.156081
H	7.285555	0.972651	1.207019
H	5.909379	1.768081	0.431009
H	7.162192	2.262858	–2.320216
H	5.541519	1.615094	–2.064718
H	6.689566	0.738776	–3.098669

E = –4430.569520, *H* = –4430.508305, *G* = –4430.652197 a.u.

NTCOOH/PCA2R

C	–4.030788	5.019337	–2.156263
C	–4.676124	5.049140	–0.944395
C	–4.801488	3.859485	–0.158265
C	–4.583152	3.858983	1.275796
C	–4.266991	2.623673	1.900933
C	–3.239409	2.589697	2.903393
C	–2.646073	1.321315	3.217159
C	–1.237345	1.266880	3.399738
C	–0.580627	0.011024	3.293220
C	0.678453	–0.040587	2.603373
C	1.127263	–1.285505	2.093424
C	1.812589	–1.312312	0.846774
C	1.957188	–2.590183	0.179414
C	1.771824	–2.603416	–1.256307
C	1.380737	–3.820203	–1.874691
C	0.337904	–3.771374	–2.868618
C	–0.389281	–4.940282	–3.277753
C	–1.745629	–4.881665	–3.463650
C	–4.228263	5.046440	1.988630
C	–3.243513	5.012469	2.948328
C	–2.567457	3.791176	3.250210
C	–1.125084	3.735333	3.438977
C	–0.482533	2.480224	3.267770
C	0.785428	2.424965	2.600653
C	1.224221	1.160305	2.083469
C	1.911897	1.122600	0.837003
C	2.047286	–0.104896	0.165110
C	2.208412	–0.111423	–1.363745
C	1.516869	–1.363614	–1.907477
C	0.441443	–1.300802	–2.796978
C	–0.266579	–2.514680	–3.119713
C	–1.686632	–2.455053	–3.321885
C	–2.454020	–3.651543	–3.263110
C	–3.743734	–3.599944	–2.612431
C	–4.394215	–4.772612	–2.107959

(CC) 2018 SCS.

C	–5.040151	–4.742722	–0.896508
C	–0.299138	4.892507	3.354152
C	0.928618	4.836012	2.726346
C	1.396921	3.621476	2.149970
C	2.102414	3.588945	0.870505
C	2.154103	2.379912	0.156967
C	1.959840	2.396912	–1.277924
C	1.607965	1.175036	–1.916865
C	0.531825	1.188892	–2.802933
C	–0.165352	–0.033312	–3.117427
C	–1.561751	0.018342	–3.295080
C	–2.333120	–1.188121	–3.192491
C	–3.605761	–1.135481	–2.574671
C	–4.180940	–2.354520	–2.087842
C	–4.862137	–2.323294	–0.823324
C	–5.078280	–3.539257	–0.122274
C	–4.863830	–3.540604	1.312352
C	–4.601957	–4.744090	2.038414
C	–3.619092	–4.775331	3.000020
C	2.324141	4.799162	0.123118
C	2.095964	4.823414	–1.225776
C	1.661843	3.635245	–1.905182
C	0.615832	3.658607	–2.897134
C	–0.082145	2.449825	–3.138005
C	–1.501969	2.494897	–3.343170
C	–2.240820	1.280472	–3.203234
C	–3.513879	1.328906	–2.586641
C	–4.088654	0.118776	–2.090961
C	–4.764466	0.150113	–0.838912
C	–4.932566	–1.074124	–0.124151
C	–4.727319	–1.073473	1.281085
C	–4.455365	–2.326482	1.925667
C	–3.429302	–2.360567	2.929589
C	–2.851698	–3.606223	3.289970
C	–1.409125	–3.659268	3.478322
C	–0.675380	–4.877566	3.401825
C	0.550967	–4.921537	2.770492
C	–0.021376	4.875675	–3.316139
C	–1.378009	4.917477	–3.505046
C	–2.177542	3.745831	–3.296799
C	–3.468924	3.796660	–2.648803
C	–3.997281	2.592322	–2.112550
C	–4.677808	2.623999	–0.847602
C	–4.840266	1.390535	–0.136123
C	–4.634179	1.388463	1.269005
C	–4.370122	0.148984	1.921738
C	–3.343675	0.114972	2.921683

(CC) 2018 SCS.

C	–2.740409	–1.138060	3.230371
C	–1.331660	–1.189717	3.413066
C	–0.672483	–2.459008	3.293977
C	0.594079	–2.507781	2.624047
C	1.109553	–3.751813	2.182465
C	1.813842	–3.784826	0.902463
C	1.944451	–5.015221	0.165681
C	1.719639	–5.033058	–1.183540
H	2.112231	5.774012	–1.748266
H	2.525504	5.730110	0.641456
H	1.460587	5.764300	2.548622
H	–0.690261	5.862724	3.640972
H	–2.881931	5.950096	3.356978
H	–4.612936	6.008959	1.669067
H	–4.956349	6.009432	–0.524674
H	–3.821361	5.956274	–2.661104
H	–1.854655	5.875441	–3.683454
H	0.545370	5.800018	–3.349849
H	–2.293352	–5.802631	–3.632940
H	0.106579	–5.904658	–3.304171
H	1.664946	–5.986257	–1.698649
H	2.073245	–5.954356	0.692466
H	1.009010	–5.889486	2.598838
H	–1.140549	–5.811957	3.696928
H	–3.330976	–5.733394	3.419499
H	–5.058830	–5.677633	1.728162
H	–5.390616	–5.675564	–0.467778
H	–4.254682	–5.727269	–2.603550
C	3.690082	–0.193530	–1.835315
O	4.085720	0.250211	–2.892165
O	4.472709	–0.861122	–0.973193
H	5.406782	–0.914853	–1.309733
C	8.755581	–0.906924	0.870762
C	7.361869	–0.777943	0.262605
C	9.746433	0.206443	0.376602
O	6.417970	–0.494698	1.159635
N	9.160777	–2.292017	0.627474
S	8.949657	1.886261	0.622923
O	7.130906	–0.977317	–0.926258
C	10.057887	0.117879	–1.124889
C	11.042652	0.129856	1.195400
H	8.644570	–0.782792	1.951863
H	5.544572	–0.461969	0.717353
H	10.038253	–2.496930	1.095920
H	9.292650	–2.455003	–0.367286
H	8.858903	1.843998	1.967906
H	10.762401	0.903941	–1.409655

(CC) 2018 SCS.

H	9.159128	0.208500	–1.737228
H	10.529925	–0.843333	–1.350239
H	11.728745	0.926534	0.898346
H	11.549025	–0.826661	1.023696
H	10.848799	0.223889	2.268379

E = –4430.569350, H = –4430.508492, G = –4430.654619 a.u.

TS_{k2}

C	5.225593	–3.685542	–2.355523
C	5.955809	–3.414129	–1.224707
C	5.726760	–2.211531	–0.482997
C	5.664312	–2.202272	0.965798
C	4.993753	–1.120990	1.596741
C	4.127283	–1.390075	2.708922
C	3.156981	–0.394625	3.063111
C	1.848200	–0.827567	3.408548
C	0.780334	0.108187	3.353608
C	–0.477021	–0.328338	2.814855
C	–1.392060	0.644558	2.336712
C	–2.170728	0.351765	1.183319
C	–2.820991	1.454528	0.510307
C	–2.794837	1.444993	–0.934400
C	–2.924277	2.681341	–1.619264
C	–2.036316	2.942560	–2.723629
C	–1.820945	4.264519	–3.241307
C	–0.560051	4.675652	–3.585678
C	5.829469	–3.393265	1.739487
C	4.999225	–3.649556	2.805340
C	3.966962	–2.727498	3.157649
C	2.627769	–3.170204	3.514012
C	1.566311	–2.233900	3.394566
C	0.300781	–2.669839	2.882152
C	–0.610894	–1.675330	2.393836
C	–1.391540	–1.958288	1.237856
C	–2.038930	–0.906253	0.563854
C	–2.316170	–1.034675	–0.937530
C	–2.179094	0.338904	–1.585130
C	–1.243587	0.603138	–2.589047
C	–1.052130	1.966439	–3.017086
C	0.265682	2.398150	–3.385856
C	0.557126	3.788907	–3.445253
C	1.840648	4.235194	–2.952279
C	2.079383	5.590761	–2.554337
C	2.812016	5.863624	–1.425299
C	2.264318	–4.547244	3.560298
C	1.039137	–4.966338	3.085727
C	0.112270	–4.032824	2.540184

(CC) 2018 SCS.

C	–0.676805	–4.330747	1.349921
C	–1.232509	–3.262063	0.621441
C	–1.173581	–3.291186	–0.827273
C	–1.353825	–2.066256	–1.528448
C	–0.441444	–1.749817	–2.539945
C	–0.264495	–0.385878	–2.960869
C	1.035187	0.047452	–3.298180
C	1.331431	1.450783	–3.311221
C	2.595562	1.887633	–2.847264
C	2.745033	3.258312	–2.457423
C	3.516465	3.545730	–1.280287
C	3.352870	4.799773	–0.634892
C	3.293526	4.811878	0.814331
C	2.692925	5.887755	1.539306
C	1.865767	5.629477	2.607357
C	–0.521064	–5.581837	0.657013
C	–0.428408	–5.600883	–0.708267
C	–0.518631	–4.380610	–1.458246
C	0.355620	–4.093107	–2.566972
C	0.545086	–2.731998	–2.914293
C	1.857041	–2.287533	–3.288012
C	2.124435	–0.885392	–3.262797
C	3.387505	–0.445706	–2.798069
C	3.541347	0.916348	–2.399154
C	4.305525	1.200360	–1.231828
C	4.096636	2.446185	–0.567545
C	4.044134	2.457900	0.851442
C	3.408520	3.571219	1.495990
C	2.543802	3.302934	2.609958
C	1.599637	4.284998	3.009064
C	0.260697	3.838320	3.364491
C	–0.863526	4.713119	3.354808
C	–2.083051	4.284298	2.872776
C	1.334530	–5.031513	–3.037423
C	2.588957	–4.603643	–3.386025
C	2.934618	–3.215820	–3.296974
C	4.218181	–2.770513	–2.803306
C	4.333842	–1.427306	–2.356850
C	5.104418	–1.141584	–1.178902
C	4.887376	0.110600	–0.516985
C	4.833337	0.124157	0.901868
C	4.211393	1.228663	1.553681
C	3.344664	0.959489	2.662548
C	2.369997	1.937144	3.013766
C	1.062088	1.501061	3.358167
C	–0.014479	2.446856	3.291991
C	–1.277052	2.005988	2.776724

(CC) 2018 SCS.

C	–2.244456	2.959949	2.375582
C	–3.039009	2.665920	1.186266
C	–3.671326	3.724854	0.444110
C	–3.601570	3.738131	–0.921946
H	–0.151488	–6.524189	–1.205573
H	–0.320439	–6.490621	1.213123
H	0.854838	–6.031482	2.999161
H	3.002791	–5.296548	3.823684
H	5.039916	–4.626902	3.274198
H	6.498667	–4.175746	1.398534
H	6.600166	–4.187455	–0.820396
H	5.314751	–4.664115	–2.814593
H	3.354845	–5.341252	–3.600291
H	1.134925	–6.096180	–2.983531
H	–0.397453	5.717747	–3.839155
H	–2.628224	4.988797	–3.230129
H	–3.938957	4.616994	–1.460881
H	–4.070807	4.589844	0.961817
H	–2.872889	5.015718	2.741202
H	–0.735596	5.766659	3.578540
H	1.298697	6.448436	3.036786
H	2.752493	6.901370	1.157947
H	2.849337	6.884474	–1.060337
H	1.560147	6.403193	–3.051075
C	–3.726996	–1.563817	–1.346590
O	–4.311030	–1.592624	–2.358196
O	–4.192484	–2.921400	–0.305334
H	–3.460874	–3.244253	0.255892
C	–7.238891	–0.183965	0.981478
C	–6.085587	–0.079558	–0.047394
C	–8.483682	–0.980878	0.447819
O	–5.025823	–0.778236	0.229108
N	–7.521890	1.192821	1.399530
S	–7.937282	–2.678093	–0.143067
O	–6.200943	0.686727	–1.008031
C	–9.144148	–0.319165	–0.770163
C	–9.512316	–1.163308	1.574841
H	–6.862384	–0.732233	1.852189
H	–4.761499	–2.255393	0.236184
H	–8.337895	1.236198	2.003617
H	–7.716956	1.748389	0.569929
H	–7.438355	–3.116774	1.030624
H	–10.002349	–0.907365	–1.108140
H	–8.439738	–0.198203	–1.594152
H	–9.511072	0.673657	–0.491866
H	–10.358889	–1.761741	1.228710
H	–9.906551	–0.193617	1.900187

(CC) 2018 SCS.

H	–9.072297	–1.660258	2.445227

E = –4430.490767, H = –4430.430272, G = –4430.572828 a.u.

NTCOO/H_2OP

C	–2.606179	5.357804	–2.700632
C	–3.393045	5.577834	–1.596950
C	–3.840828	4.481321	–0.793117
C	–3.823018	4.532893	0.656088
C	–3.825132	3.302888	1.366073
C	–2.965880	3.152254	2.506286
C	–2.660679	1.821513	2.948235
C	–1.323416	1.533123	3.333432
C	–0.897778	0.177414	3.369633
C	0.411630	–0.137100	2.870184
C	0.694386	–1.471271	2.481853
C	1.527731	–1.697548	1.349773
C	1.525638	–3.021232	0.758899
C	1.521923	–3.093104	–0.687048
C	0.999804	–4.259541	–1.305245
C	0.122149	–4.091967	–2.436757
C	–0.745731	–5.138581	–2.898577
C	–2.029382	–4.853882	–3.284015
C	–3.358041	5.682427	1.367777
C	–2.535256	5.536745	2.460138
C	–2.139919	4.237087	2.901200
C	–0.770601	3.941899	3.296399
C	–0.350037	2.585525	3.266433
C	0.963391	2.267952	2.788322
C	1.229808	0.915937	2.387461
C	2.058783	0.679967	1.255638
C	2.063725	–0.594902	0.662381
C	2.413917	–0.739439	–0.827388
C	1.581314	–1.872042	–1.415074
C	0.664823	–1.679226	–2.447323
C	–0.202771	–2.767946	–2.821775
C	–1.545430	–2.471784	–3.232173
C	–2.520156	–3.507537	–3.240334
C	–3.855163	–3.187068	–2.787877
C	–4.773141	–4.191677	–2.339511
C	–5.558246	–3.971731	–1.234652
C	0.255802	4.929403	3.285392
C	1.524725	4.619929	2.840188
C	1.836208	3.308273	2.383251
C	2.688775	3.071250	1.220580
C	2.615328	1.828852	0.570992
C	2.630524	1.783533	–0.876163
C	2.151264	0.604006	–1.512960

(CC) 2018 SCS.

C	1.220157	0.746552	–2.545850
C	0.355419	–0.348105	–2.905729
C	–0.971287	–0.061945	–3.283471
C	–1.958353	–1.104330	–3.246987
C	–3.270851	–0.788564	–2.822388
C	–4.122042	–1.853323	–2.379363
C	–4.948929	–1.622467	–1.227397
C	–5.475890	–2.734738	–0.518988
C	–5.454419	–2.685092	0.930524
C	–5.514153	–3.868700	1.730326
C	–4.688646	–4.012391	2.820994
C	3.227590	4.173365	0.466485
C	3.194039	4.148672	–0.900666
C	2.649055	3.011654	–1.588631
C	1.767247	3.153019	–2.719757
C	0.897502	2.072528	–3.010355
C	–0.449976	2.355119	–3.416242
C	–1.412235	1.302843	–3.338839
C	–2.725782	1.614749	–2.913303
C	–3.575545	0.559543	–2.461451
C	–4.396105	0.788662	–1.321449
C	–4.880542	–0.339337	–0.592747
C	–4.866498	–0.287262	0.826202
C	–4.915488	–1.526019	1.549189
C	–4.054569	–1.677333	2.688104
C	–3.766698	–2.980051	3.173104
C	–2.396928	–3.272381	3.569352
C	–1.893250	–4.602341	3.648984
C	–0.620251	–4.900008	3.207634
C	1.426850	4.433518	–3.273390
C	0.138065	4.702309	–3.653386
C	–0.883673	3.706512	–3.514408
C	–2.217927	4.026311	–3.060287
C	–3.026831	2.970889	–2.561076
C	–3.854724	3.202424	–1.410285
C	–4.335969	2.064520	–0.684025
C	–4.323680	2.114343	0.735039
C	–4.379955	0.890853	1.464535
C	–3.519523	0.739593	2.600501
C	–3.201500	–0.578079	3.038396
C	–1.863663	–0.863713	3.423965
C	–1.436040	–2.233334	3.449365
C	–0.119709	–2.545107	2.974736
C	0.217253	–3.886005	2.662923
C	1.070543	–4.123935	1.500863
C	1.069425	–5.402127	0.838599
C	1.020422	–5.466109	–0.527246

(CC) 2018 SCS.

H	3.453516	5.045434	–1.453105
H	3.522826	5.086412	0.971518
H	2.235520	5.427633	2.703979
H	0.013144	5.969137	3.476672
H	–2.067733	6.420256	2.881539
H	–3.514419	6.675329	0.960005
H	–3.545631	6.597174	–1.258823
H	–2.161713	6.209005	–3.204945
H	–0.126278	5.716103	–3.934737
H	2.153760	5.238584	–3.262230
H	–2.709206	–5.672851	–3.493508
H	–0.437604	–6.174993	–2.812367
H	0.858848	–6.425826	–1.006548
H	0.953608	–6.313583	1.414605
H	–0.326545	–5.942028	3.143784
H	–2.556013	–5.420379	3.909868
H	–4.637859	–4.978294	3.312216
H	–6.088706	–4.724837	1.393599
H	–6.128986	–4.798764	–0.825933
H	–4.747499	–5.185088	–2.774147
C	3.909071	–1.058192	–1.094586
O	4.310172	–1.665206	–2.061516
O	7.049679	–2.684898	–2.531125
H	7.500696	–1.886428	–2.836372
C	6.920609	–1.031369	0.741165
C	6.100088	–0.392153	–0.374229
C	8.355532	–0.438755	0.920830
O	4.723660	–0.566021	–0.118963
N	6.813303	–2.464829	0.482891
S	8.199704	1.400321	1.259666
O	6.469674	0.159345	–1.372542
C	9.249395	–0.581176	–0.320884
C	9.025332	–1.116761	2.125847
H	6.372924	–0.830881	1.669372
H	6.121369	–2.401329	–2.459151
H	7.197893	–3.009901	1.246285
H	7.250040	–2.727578	–0.400316
H	7.736652	1.300019	2.522035
H	10.269611	–0.266559	–0.086284
H	8.883170	0.009102	–1.161393
H	9.285860	–1.630638	–0.629996
H	9.991369	–0.651567	2.334873
H	9.203289	–2.176572	1.914893
H	8.407530	–1.047384	3.027187

E = –4430.544087, H = –4430.482376, G = –4430.629133 a.u.

(CC) 2018 SCS.

NTCOOH/PCA3R

C	–3.546092	–4.907117	2.855697
C	–4.535021	–4.884805	1.903227
C	–4.840799	–3.675459	1.200978
C	–5.075571	–3.655725	–0.230340
C	–4.909079	–2.422970	–0.915587
C	–4.242122	–2.413502	–2.187072
C	–3.716418	–1.166035	–2.663154
C	–2.434199	–1.169186	–3.276831
C	–1.718099	0.054671	–3.373789
C	–0.305962	0.037650	–3.110188
C	0.337884	1.250960	–2.757419
C	1.375155	1.222426	–1.783955
C	1.781980	2.478719	–1.188047
C	2.048862	2.471827	0.235317
C	1.925235	3.692413	0.950398
C	1.238217	3.669942	2.217249
C	0.729538	4.861360	2.837091
C	–0.502303	4.858062	3.437145
C	–5.015020	–4.843038	–1.024451
C	–4.375101	–4.832575	–2.241943
C	–3.769238	–3.635973	–2.732432
C	–2.456779	–3.639066	–3.362013
C	–1.734226	–2.416675	–3.393941
C	–0.320500	–2.429848	–3.154345
C	0.316135	–1.196001	–2.791654
C	1.355131	–1.213027	–1.818284
C	1.748959	–0.006955	–1.213383
C	2.374161	–0.036557	0.188294
C	1.945259	1.232064	0.926712
C	1.196541	1.199214	2.105199
C	0.682429	2.436228	2.637965
C	–0.605146	2.434312	3.272895
C	–1.295077	3.663810	3.463112
C	–2.724547	3.680848	3.248284
C	–3.443817	4.890222	2.977739
C	–4.433702	4.912171	2.026212
C	–1.701123	–4.832417	–3.545176
C	–0.337760	–4.841745	–3.331136
C	0.343303	–3.660413	–2.922000
C	1.410818	–3.683904	–1.923946
C	1.736249	–2.492838	–1.254182
C	1.994290	–2.530158	0.170326
C	1.913845	–1.307331	0.893535
C	1.166584	–1.291950	2.070253
C	0.660177	–0.046975	2.592028
C	–0.611981	–0.041513	3.196366

(CC) 2018 SCS.

C	–1.318841	1.199238	3.345777
C	–2.721622	1.213893	3.155799
C	–3.361449	2.466147	2.878949
C	–4.401149	2.489434	1.887550
C	–4.765266	3.727339	1.294437
C	–5.002764	3.748397	–0.136384
C	–4.920255	4.954038	–0.900323
C	–4.282036	4.961997	–2.118677
C	1.796277	–4.917091	–1.288560
C	1.994182	–4.958587	0.064755
C	1.846773	–3.766824	0.852136
C	1.158873	–3.764549	2.119239
C	0.628611	–2.531613	2.572689
C	–0.657278	–2.519077	3.210129
C	–1.344690	–1.271127	3.314414
C	–2.747221	–1.252042	3.125
C	–3.389759	–0.008468	2.839501
C	–4.420340	0.014395	1.858171
C	–4.742319	1.258790	1.236990
C	–4.980209	1.277548	–0.162970
C	–4.861177	2.530356	–0.852939
C	–4.195388	2.540114	–2.125081
C	–3.699415	3.766695	–2.639742
C	–2.386596	3.760678	–3.268616
C	–1.607787	4.943717	–3.418853
C	–0.245055	4.921423	–3.201813
C	0.625455	–4.961231	2.707270
C	–0.604946	–4.947913	3.310284
C	–1.372293	–3.738299	3.369937
C	–2.802071	–3.720045	3.156343
C	–3.413239	–2.483568	2.817590
C	–4.452231	–2.460561	1.825380
C	–4.767401	–1.207221	1.205861
C	–5.004432	–1.185893	–0.194172
C	–4.895753	0.053858	–0.889527
C	–4.229134	0.063380	–2.158200
C	–3.693197	1.295134	–2.632411
C	–2.410906	1.289219	–3.245796
C	–1.687436	2.525918	–3.330961
C	–0.274400	2.505924	–3.088772
C	0.412258	3.716826	–2.822794
C	1.479731	3.692914	–1.824920
C	1.891285	4.901222	–1.158113
C	2.093795	4.902385	0.194794
H	2.127442	–5.919326	0.550699
H	1.784920	–5.845293	–1.849276
H	0.178394	–5.795587	–3.333100

(CC) 2018 SCS.

H	–2.207492	–5.778865	–3.701198
H	–4.202391	–5.776689	–2.747609
H	–5.327358	–5.794074	–0.606667
H	–4.976046	–5.823690	1.585806
H	–3.235591	–5.862085	3.265693
H	–1.048551	–5.887837	3.621068
H	1.128725	–5.910045	2.555066
H	–0.926141	5.798483	3.773014
H	1.253470	5.802795	2.711443
H	2.247876	5.846622	0.706225
H	1.898471	5.843823	–1.694313
H	0.289075	5.865013	–3.177282
H	–2.095706	5.903468	–3.550491
H	–4.091623	5.915079	–2.600610
H	–5.213501	5.899957	–0.457804
H	–4.855239	5.867682	1.732813
H	–3.113262	5.828073	3.410885
C	3.932499	–0.033494	0.187356
O	4.588123	–0.388677	1.149475
O	4.455642	0.427988	–0.948514
H	5.441618	0.444229	–0.870898
C	10.004013	–0.718580	–0.066520
C	10.759832	0.600758	–0.221302
C	8.473359	–0.511270	0.226348
O	11.177172	0.812905	–1.481447
N	10.743418	–1.483071	0.938205
S	7.751331	0.620086	–1.092168
O	11.001575	1.363243	0.694136
C	8.198772	0.200056	1.559509
C	7.750852	–1.864705	0.184417
H	10.081210	–1.256913	–1.015858
H	11.656385	1.661144	–1.491483
H	10.331642	–2.402567	1.066852
H	10.717492	–1.002165	1.833652
H	7.943735	–0.187066	–2.155211
H	7.121214	0.304768	1.707883
H	8.670660	1.183230	1.604316
H	8.590711	–0.403431	2.384119
H	6.682537	–1.727481	0.363620
H	8.136799	–2.523086	0.970600
H	7.887696	–2.368362	–0.777528

E = –4430.565697, H = –4430.504710, G = –4430.652141 a.u.

(CC) 2018 SCS.

TS_{k3}

C	5.653847	–3.122662	–2.259103
C	6.336480	–2.736084	–1.132095
C	5.953101	–1.555525	–0.419262
C	5.879430	–1.522258	1.028887
C	5.073075	–0.520603	1.631731
C	4.239686	–0.872057	2.746137
C	3.149387	0.000614	3.073589
C	1.903630	–0.585735	3.425634
C	0.726586	0.206252	3.346439
C	–0.463793	–0.397918	2.816874
C	–1.491132	0.440731	2.313681
C	–2.219989	0.025078	1.165199
C	–2.993077	1.025231	0.461933
C	–2.953780	0.985441	–0.981058
C	–3.240159	2.176561	–1.697778
C	–2.386204	2.522621	–2.806011
C	–2.336902	3.848892	–3.353905
C	–1.135771	4.409000	–3.702543
C	6.187335	–2.665742	1.830070
C	5.388480	–3.000985	2.898283
C	4.246596	–2.208181	3.225888
C	2.971785	–2.807633	3.589939
C	1.801077	–2.016094	3.445678
C	0.602479	–2.620433	2.942881
C	–0.425777	–1.761189	2.428469
C	–1.160179	–2.168432	1.279435
C	–1.933320	–1.223653	0.577012
C	–2.171639	–1.414560	–0.924425
C	–2.198167	–0.049892	–1.600137
C	–1.302176	0.307132	–2.610441
C	–1.283925	1.673017	–3.071939
C	–0.029206	2.259772	–3.446602
C	0.083883	3.674519	–3.537043
C	1.297356	4.290801	–3.049011
C	1.358833	5.673706	–2.680452
C	2.045393	6.062916	–1.556573
C	2.785027	–4.217947	3.670202
C	1.624798	–4.799734	3.204175
C	0.590579	–4.003901	2.633628
C	–0.145747	–4.426282	1.447896
C	–0.827448	–3.452694	0.693208
C	–0.749405	–3.503587	–0.754172
C	–1.079898	–2.326463	–1.482970
C	–0.209737	–1.922509	–2.501775
C	–0.204127	–0.558508	–2.956015
C	1.031947	0.028142	–3.301512

(CC) 2018 SCS.

C	1.147738	1.456982	–3.346104
C	2.343555	2.060905	–2.888152
C	2.314995	3.447684	–2.528658
C	3.037509	3.857039	–1.356878
C	2.713347	5.094703	–0.740826
C	2.644817	5.131896	0.707673
C	1.909652	6.139508	1.406487
C	1.114313	5.802225	2.476679
C	0.173544	–5.661727	0.783754
C	0.279070	–5.698391	–0.580346
C	0.041285	–4.516212	–1.357738
C	0.878164	–4.145957	–2.470507
C	0.895133	–2.780456	–2.849637
C	2.141855	–2.182841	–3.232588
C	2.230033	–0.758045	–3.240902
C	3.424915	–0.151423	–2.783174
C	3.401961	1.227487	–2.414832
C	4.117268	1.632079	–1.252158
C	3.748591	2.856155	–0.617304
C	3.685507	2.892565	0.800795
C	2.910463	3.930828	1.417527
C	2.078961	3.579992	2.533686
C	1.016655	4.444053	2.907161
C	–0.257197	3.840726	3.269330
C	–1.481905	4.567133	3.235738
C	–2.634966	3.977765	2.759723
C	1.969131	–4.963941	–2.917860
C	3.160973	–4.389381	–3.275336
C	3.328056	–2.967488	–3.218146
C	4.542401	–2.352264	–2.731831
C	4.484738	–0.995481	–2.316069
C	5.205212	–0.588600	–1.142275
C	4.827789	0.640933	–0.510178
C	4.762144	0.678726	0.907755
C	4.001460	1.710105	1.531606
C	3.167504	1.357966	2.642346
C	2.075762	2.212652	2.967963
C	0.831208	1.623159	3.318692
C	–0.355150	2.424347	3.228210
C	–1.549184	1.816466	2.720236
C	–2.625317	2.632760	2.293207
C	–3.366963	2.214711	1.107614
C	–4.126349	3.164695	0.337812
C	–4.054015	3.152474	–1.028471
H	0.675230	–6.589478	–1.055148
H	0.483636	–6.525396	1.361045
H	1.576572	–5.881375	3.143132

(CC) 2018 SCS.

H	3.610991	–4.861226	3.953406
H	5.547169	–3.955527	3.388566
H	6.951164	–3.365699	1.509133
H	7.069703	–3.413154	–0.707106
H	5.868213	–4.092671	–2.694323
H	4.014521	–5.029275	–3.471940
H	1.904965	–6.043730	–2.839432
H	–1.105089	5.457538	–3.978996
H	–3.229368	4.465105	–3.361763
H	–4.500931	3.965695	–1.590154
H	–4.637448	3.982765	0.833172
H	–3.509359	4.600998	2.607269
H	–1.487961	5.633323	3.434751
H	0.446054	6.552307	2.886020
H	1.844376	7.144184	1.003037
H	1.949936	7.087892	–1.214487
H	0.742209	6.401974	–3.195860
C	–3.507621	–2.133306	–1.353854
O	–4.035790	–2.185737	–2.405486
O	–3.731753	–3.598242	–0.467627
H	–2.958556	–3.834512	0.085517
C	–8.168559	–1.440939	0.600889
C	–8.031290	–0.163405	1.426058
C	–6.992620	–1.643799	–0.422193
O	–7.845919	–0.404623	2.738395
N	–9.524995	–1.387304	0.036341
S	–5.389215	–1.550848	0.549386
O	–8.142303	0.963669	0.980442
C	–6.980892	–0.565582	–1.518278
C	–7.146985	–3.034808	–1.060698
H	–8.134274	–2.283548	1.297094
H	–7.796904	0.460306	3.183732
H	–9.719921	–2.237971	–0.484689
H	–9.590243	–0.612533	–0.619754
H	–4.465575	–3.142132	0.142643
H	–6.156391	–0.748014	–2.210694
H	–6.868716	0.434102	–1.096025
H	–7.911643	–0.591061	–2.099136
H	–6.321839	–3.234588	–1.747301
H	–8.076375	–3.101391	–1.640118
H	–7.161217	–3.821808	–0.299911

E = –4430.483108, H = –4430.422702, G = –4430.565815 a.u.

(CC) 2018 SCS.

NTCOS/H_2OP

C	4.406336	–4.315808	–2.562337
C	5.216613	–4.190293	–1.460930
C	5.213678	–2.983765	–0.690303
C	5.212222	–2.997615	0.759928
C	4.747228	–1.838541	1.436267
C	3.891877	–1.991505	2.579147
C	3.106190	–0.862767	2.988262
C	1.758451	–1.089382	3.378342
C	0.852713	0.006093	3.382975
C	–0.478075	–0.211438	2.889443
C	–1.242856	0.906306	2.467681
C	–2.097943	0.768080	1.339449
C	–2.593244	1.976360	0.713226
C	–2.619325	1.998880	–0.733794
C	–2.582677	3.256853	–1.393772
C	–1.702797	3.400475	–2.528534
C	–1.294595	4.684224	–3.025538
C	0.003329	4.896042	–3.410581
C	5.213859	–4.217064	1.506515
C	4.393899	–4.362219	2.601088
C	3.535713	–3.296298	3.010257
C	2.156000	–3.528395	3.411079
C	1.254400	–2.432505	3.350287
C	–0.082763	–2.648192	2.880637
C	–0.840635	–1.509334	2.446909
C	–1.698013	–1.637393	1.318648
C	–2.186779	–0.477334	0.688030
C	–2.552571	–0.524460	–0.801616
C	–2.206761	0.824541	–1.423908
C	–1.288594	0.962827	–2.465543
C	–0.897976	2.287804	–2.877268
C	0.458024	2.510608	–3.290684
C	0.967391	3.837912	–3.334284
C	2.323647	4.059642	–2.886780
C	2.792158	5.349375	–2.474413
C	3.602749	5.474576	–1.373297
C	1.578780	–4.830183	3.438916
C	0.286146	–5.035710	3.002263
C	–0.498388	–3.952614	2.514265
C	–1.376483	–4.089195	1.354985
C	–1.777020	–2.930129	0.670181
C	–1.798818	–2.935034	–0.777670
C	–1.795387	–1.679743	–1.448095
C	–0.881584	–1.493814	–2.487140
C	–0.495887	–0.163935	–2.887196
C	0.839950	0.062595	–3.271538

(CC) 2018 SCS.

C	1.358068	1.401719	–3.272837
C	2.692267	1.618525	–2.853268
C	3.075678	2.938261	–2.446310
C	3.928332	3.070407	–1.297899
C	3.995043	4.319098	–0.624652
C	3.994508	4.306399	0.825459
C	3.603341	5.447308	1.593452
C	2.783510	5.299522	2.687616
C	–1.457439	–5.334043	0.636115
C	–1.430829	–5.338086	–0.731589
C	–1.350809	–4.100054	–1.455142
C	–0.477862	–3.931757	–2.589333
C	–0.081446	–2.612032	–2.919387
C	1.272592	–2.375532	–3.332720
C	1.764696	–1.035273	–3.294297
C	3.098456	–0.814220	–2.875285
C	3.484571	0.496905	–2.459912
C	4.329736	0.627770	–1.322686
C	4.350640	1.875411	–0.628980
C	4.355888	1.862171	0.790825
C	3.932675	3.047562	1.479982
C	3.077006	2.894782	2.622485
C	2.318504	4.005887	3.075306
C	0.939165	3.771444	3.475103
C	–0.028850	4.815313	3.522906
C	–1.319133	4.598193	3.085265
C	0.323162	–5.004531	–3.108928
C	1.617482	–4.777014	–3.496264
C	2.185536	–3.464337	–3.398759
C	3.542152	–3.241440	–2.952674
C	3.891175	–1.944500	–2.490784
C	4.743483	–1.812746	–1.341923
C	4.756623	–0.557443	–0.650789
C	4.761117	–0.568138	0.769100
C	4.349441	0.606033	1.464949
C	3.493369	0.453104	2.603648
C	2.701210	1.565270	3.009704
C	1.354028	1.336057	3.399773
C	0.441579	2.443546	3.393142
C	–0.894282	2.222068	2.922728
C	–1.711400	3.327428	2.577435
C	–2.588292	3.191470	1.417452
C	–3.073505	4.353847	0.719449
C	–3.057789	4.389558	–0.647907
H	–1.331113	–6.282409	–1.256130
H	–1.387175	–6.275983	1.168762
H	–0.067237	–6.055557	2.896307

(CC) 2018 SCS.

H	2.196984	–5.694962	3.654363
H	4.293769	–5.344575	3.050303
H	5.734988	–5.088462	1.124964
H	5.744340	–5.065594	–1.097469
H	4.318205	–5.285577	–3.040099
H	2.246812	–5.623059	–3.750927
H	–0.044167	–6.024204	–3.066184
H	0.323219	5.905452	–3.646097
H	–1.972746	5.528682	–2.965852
H	–3.274599	5.323217	–1.155726
H	–3.311097	5.258252	1.268510
H	–1.984460	5.449940	2.995191
H	0.276077	5.829970	3.755137
H	2.372074	6.188183	3.154284
H	3.813490	6.447109	1.229234
H	3.818017	6.467275	–0.992521
H	2.391741	6.245994	–2.935041
C	–4.080800	–0.753635	–1.116254
O	–4.469541	–0.777448	–2.270703
O	–4.973508	1.669468	–3.743544
H	–4.695834	2.279443	–3.046900
C	–7.783650	–1.255831	0.921164
C	–7.621109	–0.147073	1.962158
C	–6.881772	–1.034136	–0.363040
O	–6.838212	–0.517466	2.990755
N	–9.216357	–1.347429	0.659487
S	–5.118852	–0.938070	0.317416
O	–8.150945	0.943560	1.888812
C	–7.234515	0.265012	–1.099748
C	–7.016838	–2.263344	–1.274223
H	–7.461576	–2.194196	1.382316
H	–6.769158	0.242030	3.597423
H	–9.417178	–2.077205	–0.017091
H	–9.561290	–0.466973	0.286431
H	–4.669954	0.808186	–3.415223
H	–6.575063	0.431280	–1.952022
H	–7.179147	1.130164	–0.436597
H	–8.258396	0.195925	–1.482772
H	–6.347249	–2.179882	–2.129466
H	–8.039517	–2.329764	–1.659806
H	–6.790334	–3.187066	–0.734056

E = –4430.547331, H = –4430.485326, G = –4430.633099 a.u.

(CC) 2018 SCS.

In DMF

NTCOCl

C	4.900760	–2.441822	2.819045
C	4.900987	–3.381920	1.818167
C	3.703849	–3.665381	1.086368
C	3.704553	–3.829080	–0.354755
C	2.478749	–3.641934	–1.046928
C	2.478488	–2.913822	–2.284288
C	1.232018	–2.377139	–2.749990
C	1.229890	–1.066096	–3.298558
C	0.000109	–0.357690	–3.376089
C	–0.000564	1.038786	–3.041224
C	–1.225162	1.654780	–2.677203
C	–1.220406	2.643932	–1.654577
C	–2.487959	3.006744	–1.056346
C	–2.502774	3.196521	0.378461
C	–3.731020	3.027497	1.070644
C	–3.717378	2.278289	2.302210
C	–4.911300	1.728962	2.880779
C	–4.902513	0.469377	3.420012
C	4.901089	–3.719266	–1.129400
C	4.899421	–3.021168	–2.314444
C	3.702845	–2.403480	–2.790196
C	3.700536	–1.061707	–3.353696
C	2.471547	–0.349952	–3.365589
C	2.467828	1.049739	–3.055533
C	1.223469	1.656072	–2.677479
C	1.217916	2.645289	–1.654888
C	–0.001362	3.004363	–1.050772
C	–0.001412	3.540558	0.380362
C	–1.271873	3.067130	1.080875
C	–1.245013	2.264653	2.222749
C	–2.483756	1.714418	2.712567
C	–2.476102	0.398569	3.285584
C	–3.700415	–0.311720	3.425097
C	–3.699435	–1.728951	3.140095
C	–4.897543	–2.446487	2.819701
C	–4.897000	–3.386621	1.818855
C	4.888710	–0.286750	–3.485282
C	4.881997	1.063702	–3.202789
C	3.688818	1.712127	–2.774760
C	3.688924	2.727395	–1.724549
C	2.485227	3.009312	–1.056841
C	2.500138	3.198823	0.378004
C	1.269513	3.068131	1.080589
C	1.243638	2.265699	2.222456
C	–0.000398	1.722452	2.703954

(CC) 2018 SCS.

C	0.000260	0.420702	3.243326
C	–1.234364	–0.305007	3.341060
C	–1.231669	–1.696318	3.080078
C	–2.473386	–2.334173	2.755635
C	–2.473217	–3.323191	1.713682
C	–3.699690	–3.668968	1.086902
C	–3.700432	–3.832746	–0.354210
C	–4.897186	–3.724159	–1.128688
C	–4.896378	–3.026094	–2.313748
C	4.908975	3.093508	–1.054030
C	4.929512	3.226006	0.307743
C	3.728672	3.030974	1.069961
C	3.715986	2.281730	2.301525
C	2.482981	1.716697	2.712119
C	2.476665	0.400895	3.285220
C	1.235595	–0.303846	3.340891
C	1.234199	–1.695155	3.079922
C	0.001548	–2.335678	2.747728
C	0.001953	–3.315594	1.715285
C	–1.231120	–3.619353	1.063148
C	–1.229920	–3.785598	–0.347145
C	–2.474913	–3.644407	–1.046568
C	–2.475547	–2.916322	–2.283940
C	–3.700489	–2.407212	–2.789669
C	–3.699619	–1.065433	–3.353135
C	–4.888596	–0.291660	–3.484474
C	–4.883188	1.058779	–3.201890
C	4.910534	1.733583	2.879925
C	4.903033	0.474032	3.419258
C	3.701677	–0.308212	3.424583
C	3.702009	–1.725444	3.139614
C	2.476486	–2.331829	2.755317
C	2.477131	–3.320822	1.713341
C	1.235228	–3.618159	1.062972
C	1.233997	–3.784379	–0.347325
C	0.001923	–3.653953	–1.052331
C	0.001476	–2.924591	–2.285792
C	–1.229681	–2.378383	–2.749818
C	–1.228953	–1.067336	–3.298373
C	–2.471345	–0.352447	–3.365196
C	–2.468983	1.047220	–3.055058
C	–3.690582	1.708371	–2.774036
C	–3.691497	2.723639	–1.723824
C	–4.911787	3.088648	–1.053129
C	–4.932199	3.221268	0.308630
H	5.882025	3.342802	0.813541
H	5.845183	3.116737	–1.600683

(CC) 2018 SCS.

H	5.830217	1.588981	–3.168520
H	5.841692	–0.775791	–3.655670
H	5.847863	–2.815423	–2.799210
H	5.849800	–4.042592	–0.714851
H	5.848281	–3.797596	1.491571
H	5.846957	–2.142825	3.256803
H	5.843782	0.025675	3.720554
H	5.855180	2.254463	2.766986
H	–5.842784	0.020092	3.721417
H	–5.856466	2.248933	2.768001
H	–5.884732	3.337167	0.814598
H	–5.848116	3.110927	–1.599616
H	–5.831923	1.583113	–3.167437
H	–5.841117	–0.781645	–3.654737
H	–5.845090	–2.821292	–2.798381
H	–5.845517	–4.048406	–0.713990
H	–5.843937	–3.803222	1.492408
H	–5.843966	–2.148394	3.257588
C	–0.002142	5.107084	0.524330
O	0.002021	5.700775	1.552773
Cl	–0.012181	6.053417	–1.054932

E = –4014.510336, H = –4014.462844, G = –4014.576271 a.u.

PCA

C	–0.414409	0.595877	–0.596904
C	–1.590553	–0.142104	0.041917
C	0.965671	0.211041	0.048639
O	–2.173835	–1.013997	–0.799436
N	–0.770706	2.015061	–0.554346
S	1.156491	–1.654182	0.029324
O	–1.998427	0.062730	1.168897
C	1.073434	0.617554	1.526115
C	2.104467	0.846632	–0.761815
H	–0.371058	0.298438	–1.648926
H	–2.918564	–1.423393	–0.322931
H	–0.063374	2.578991	–1.016145
H	–0.840297	2.330224	0.409649
H	1.117899	–1.821457	–1.308561
H	2.052106	0.336056	1.924426
H	0.294593	0.156450	2.135572
H	0.980608	1.704134	1.618434
H	3.074041	0.548334	–0.356036
H	2.046387	1.939710	–0.713121
H	2.065192	0.550127	–1.814521

E = –800.416896, H = –800.404947, G = –800.452897 a.u.

(CC) 2018 SCS.

NTCOCl/PCA1R

C	0.330914	5.258233	3.202813
C	1.490324	5.713761	2.625082
C	2.457537	4.791581	2.111953
C	3.114620	4.998287	0.835373
C	3.678787	3.868305	0.186156
C	3.505823	3.717141	–1.230946
C	3.701271	2.414010	–1.798453
C	2.788726	1.972217	–2.794603
C	2.692737	0.580688	–3.067285
C	1.387949	0.019099	–3.277821
C	1.209523	–1.377554	–3.105629
C	–0.000570	–1.849661	–2.526970
C	–0.031330	–3.212599	–2.040143
C	–0.709007	–3.441435	–0.782207
C	–0.340951	–4.577262	–0.013781
C	–0.156923	–4.405031	1.405271
C	0.560008	–5.355612	2.207683
C	1.431548	–4.926562	3.174220
C	2.836154	6.135512	0.015074
C	2.670378	5.989084	–1.342490
C	2.781029	4.702175	–1.951774
C	1.847597	4.249973	–2.973088
C	1.724481	2.851103	–3.186513
C	0.427590	2.287908	–3.423320
C	0.257939	0.875083	–3.236760
C	–0.951266	0.392455	–2.660735
C	–1.001196	–0.925766	–2.170593
C	–1.971806	–1.264686	–1.036509
C	–1.332681	–2.330564	–0.147296
C	–1.073429	–2.115288	1.209329
C	–0.303549	–3.096990	1.931026
C	0.603744	–2.651574	2.950256
C	1.629088	–3.525867	3.405647
C	2.934437	–2.962945	3.667287
C	4.121754	–3.764256	3.696366
C	5.281673	–3.308192	3.119986
C	0.778563	5.064781	–3.444589
C	–0.465453	4.520411	–3.688712
C	–0.708285	3.133862	–3.474685
C	–1.949636	2.645535	–2.879337
C	–1.964637	1.363816	–2.303379
C	–2.642385	1.166538	–1.040181
C	–2.305182	0.014329	–0.276595
C	–2.028354	0.178843	1.079822
C	–1.264518	–0.812685	1.792783
C	–0.355617	–0.375775	2.777423

(CC) 2018 SCS.

C	0.701463	–1.248953	3.200527
C	1.975236	–0.696258	3.476825
C	3.113451	–1.566976	3.475327
C	4.329347	–1.088955	2.878115
C	5.323410	–2.024723	2.487347
C	5.984036	–1.817485	1.212774
C	6.636736	–2.880972	0.514954
C	6.473207	–3.023649	–0.843159
C	–2.972277	3.564807	–2.454319
C	–3.582388	3.398929	–1.240589
C	–3.225289	2.291726	–0.399416
C	–3.028241	2.440290	1.021564
C	–2.220009	1.477343	1.674901
C	–1.310779	1.908728	2.697561
C	–0.253512	1.025156	3.074394
C	1.021071	1.574085	3.351782
C	2.161100	0.713640	3.344728
C	3.365680	1.187607	2.752538
C	4.335240	0.232210	2.322655
C	4.984624	0.438181	1.076654
C	5.599294	–0.690641	0.438849
C	5.428880	–0.841039	–0.978605
C	5.655485	–2.109243	–1.574562
C	4.720866	–2.558842	–2.595649
C	4.572732	–3.932612	–2.942241
C	3.323081	–4.466365	–3.180911
C	–3.234626	3.688560	1.700297
C	–2.359545	4.101660	2.670616
C	–1.233848	3.289554	3.028699
C	0.071087	3.852185	3.293865
C	1.198217	2.990892	3.225739
C	2.413635	3.469236	2.627687
C	3.380504	2.502867	2.197455
C	4.029945	2.706034	0.951082
C	4.650003	1.593356	0.311459
C	4.475813	1.441763	–1.102816
C	4.657004	0.149159	–1.673208
C	3.743357	–0.290058	–2.669266
C	3.643561	–1.696969	–2.933478
C	2.343904	–2.254691	–3.165537
C	2.155658	–3.657014	–3.087269
C	0.915787	–4.146617	–2.490493
C	0.836534	–5.475122	–1.941436
C	0.236859	–5.680271	–0.729027
H	–4.230697	4.182576	–0.863268
H	–3.155201	4.473053	–3.017717
H	–1.290662	5.191546	–3.900550

(CC) 2018 SCS.

H	0.885974	6.143821	–3.467183
H	2.302456	6.833075	–1.916157
H	2.593840	7.089310	0.471088
H	1.594369	6.775576	2.428919
H	–0.447542	5.972142	3.449463
H	–2.451751	5.106742	3.068026
H	–4.000182	4.373890	1.352763
H	2.067236	–5.653215	3.668877
H	0.524160	–6.410734	1.958877
H	0.323399	–6.651094	–0.252916
H	1.379033	–6.290272	–2.407444
H	3.233159	–5.541377	–3.292267
H	5.419091	–4.606825	–2.868528
H	6.843881	–3.924229	–1.320996
H	7.130922	–3.672506	1.067831
H	6.118854	–3.990524	3.019112
H	4.075295	–4.793023	4.036754
C	–3.351701	–1.871322	–1.473651
O	–4.318919	–1.928723	–0.781566
C	–8.024416	–1.344557	0.743795
C	–9.296075	–1.884004	1.398809
C	–8.294854	–0.085872	–0.157253
O	–9.289356	–1.741944	2.736864
N	–7.404787	–2.491756	0.081479
S	–9.245496	1.190349	0.837145
O	–10.200031	–2.433772	0.799341
C	–9.177773	–0.397971	–1.374784
C	–6.958670	0.518398	–0.610516
H	–7.353237	–1.024683	1.546543
H	–10.117415	–2.129351	3.073509
H	–6.492819	–2.253515	–0.297976
H	–7.992764	–2.820387	–0.679474
H	–8.318547	1.386658	1.797084
H	–9.344158	0.507795	–1.964444
H	–10.142695	–0.816787	–1.084401
H	–8.671530	–1.121729	–2.021100
H	–7.130040	1.415850	–1.210010
H	–6.404942	–0.197199	–1.226837
H	–6.327303	0.789603	0.241175
Cl	–3.418449	–2.577038	–3.158963

E = –4814.929407, H = –4814.867543, G = –4815.019648 a.u.

(CC) 2018 SCS.

TS_{k4}

C	–2.073092	–5.032114	3.322016
C	–3.290242	–5.087987	2.688281
C	–3.863406	–3.911468	2.109190
C	–4.496038	–3.927624	0.803558
C	–4.614516	–2.696527	0.105707
C	–4.338209	–2.661632	–1.302734
C	–4.053249	–1.389605	–1.901926
C	–2.999954	–1.317533	–2.853620
C	–2.423042	–0.051742	–3.143184
C	–0.996217	0.026975	–3.292327
C	–0.361090	1.284669	–3.133115
C	0.913753	1.339075	–2.501900
C	1.372141	2.627847	–2.029424
C	2.033212	2.654482	–0.746298
C	2.043264	3.873044	–0.019361
C	1.754525	3.822344	1.391150
C	1.372131	4.985726	2.140624
C	0.362868	4.911382	3.064669
C	–4.584546	–5.119309	0.018774
C	–4.319845	–5.084221	–1.330658
C	–3.960352	–3.857609	–1.967388
C	–2.885417	–3.783430	–2.946461
C	–2.282393	–2.517606	–3.173646
C	–0.861810	–2.435900	–3.349157
C	–0.227823	–1.159166	–3.175199
C	1.048817	–1.096157	–2.546769
C	1.528851	0.143665	–2.079817
C	2.520261	0.174761	–0.901134
C	2.240628	1.417006	–0.070248
C	1.845381	1.352480	1.274038
C	1.423194	2.559988	1.941676
C	0.373002	2.485057	2.916835
C	–0.312019	3.670257	3.304393
C	–1.742063	3.593663	3.502286
C	–2.585216	4.750765	3.452834
C	–3.803787	4.695729	2.821673
C	–2.139342	–4.927835	–3.349435
C	–0.774445	–4.846709	–3.534362
C	–0.083279	–3.619496	–3.325996
C	1.219151	–3.563125	–2.668185
C	1.644374	–2.343949	–2.113930
C	2.286387	–2.343817	–0.820701
C	2.341781	–1.114222	–0.102953
C	1.964549	–1.129595	1.240871
C	1.554352	0.085771	1.894028
C	0.506733	0.016828	2.836582

(CC) 2018 SCS.

C	–0.208372	1.209241	3.185980
C	–1.605530	1.131399	3.402696
C	–2.377567	2.335917	3.323728
C	–3.655079	2.278305	2.669979
C	–4.252954	3.481680	2.210840
C	–4.890357	3.466348	0.907970
C	–5.111149	4.662969	0.157519
C	–4.850001	4.694163	–1.192520
C	1.843335	–4.760091	–2.170652
C	2.419400	–4.767274	–0.929428
C	2.427433	–3.574592	–0.130934
C	2.135656	–3.597240	1.281886
C	1.676580	–2.394874	1.871900
C	0.630360	–2.456322	2.850942
C	–0.079449	–1.254309	3.152864
C	–1.476241	–1.329393	3.369998
C	–2.254097	–0.135077	3.285475
C	–3.520426	–0.193019	2.636872
C	–4.086857	1.018758	2.139334
C	–4.714183	1.001871	0.865365
C	–4.879923	2.249447	0.175792
C	–4.606658	2.283637	–1.233172
C	–4.361148	3.531702	–1.862980
C	–3.284558	3.601716	–2.839893
C	–2.663918	4.831064	–3.203780
C	–1.297435	4.901730	–3.380843
C	1.877027	–4.815689	1.994613
C	0.871409	–4.873509	2.924409
C	0.074158	–3.716611	3.204901
C	–1.356056	–3.794848	3.405346
C	–2.118846	–2.606070	3.259107
C	–3.395545	–2.665011	2.603193
C	–3.956948	–1.443840	2.105370
C	–4.582813	–1.458212	0.830702
C	–4.760242	–0.224202	0.139718
C	–4.482212	–0.189580	–1.266041
C	–4.186894	1.066979	–1.867535
C	–3.132980	1.135742	–2.818727
C	–2.548991	2.415033	–3.101269
C	–1.127700	2.490880	–3.270610
C	–0.480176	3.749345	–3.205424
C	0.820941	3.810773	–2.546447
C	1.322220	5.052603	–2.018050
C	1.904537	5.082762	–0.780893
H	2.745007	–5.709944	–0.502574
H	1.729038	–5.696284	–2.705750
H	–0.219000	–5.764647	–3.693054

(CC) 2018 SCS.

H	–2.607709	–5.906103	–3.363145
H	–4.235134	–6.022082	–1.869222
H	–4.700090	–6.082992	0.502978
H	–3.738533	–6.058226	2.502712
H	–1.594872	–5.958724	3.620522
H	0.598984	–5.835814	3.344652
H	2.377379	–5.732046	1.700722
H	–0.007279	5.826651	3.514262
H	1.778085	5.956770	1.878308
H	2.134479	6.040318	–0.325846
H	1.109449	5.986557	–2.526373
H	–0.842408	5.877958	–3.507833
H	–3.234056	5.753715	–3.190962
H	–4.870432	5.650011	–1.705093
H	–5.329946	5.594078	0.669001
H	–4.352149	5.618276	2.663498
H	–2.207005	5.714120	3.777380
C	4.019206	0.078737	–1.448137
O	4.505766	–0.878105	–1.968827
C	6.447471	0.068321	–0.021907
C	6.403700	–1.440888	0.223718
C	7.465265	0.823101	0.910503
O	7.139910	–2.136199	–0.645887
N	5.063542	0.543420	0.154186
S	9.160894	0.052643	0.751933
O	5.752367	–1.942073	1.120277
C	7.102697	0.698348	2.399526
C	7.550768	2.301485	0.496403
H	6.727713	0.246917	–1.062928
H	7.078045	–3.077583	–0.403147
H	5.000032	1.554522	0.229259
H	4.648014	0.106900	0.977900
H	9.332782	0.273495	–0.567005
H	7.853917	1.207042	3.009116
H	7.037497	–0.343152	2.720679
H	6.140005	1.178278	2.599198
H	8.297268	2.812428	1.108318
H	6.597407	2.820696	0.648738
H	7.832561	2.410126	–0.554502
Cl	4.584033	1.839073	–2.442619

E = –4814.918925, H = –4814.858862, G = –4815.000569 a.u.

(CC) 2018 SCS.

NTCON/HClP

C	3.128087	5.126680	2.726726
C	4.014439	5.212113	1.681601
C	4.365315	4.046063	0.928759
C	4.457091	4.063984	–0.518399
C	4.343892	2.827717	–1.208203
C	3.554582	2.765344	–2.405844
C	3.105533	1.476977	–2.849943
C	1.771980	1.359531	–3.327257
C	1.172206	0.071821	–3.374311
C	–0.198702	–0.053001	–2.966737
C	–0.685723	–1.328576	–2.581654
C	–1.621382	–1.414275	–1.513221
C	–1.842985	–2.709766	–0.905231
C	–1.959901	–2.743121	0.538114
C	–1.644318	–3.952865	1.211436
C	–0.836315	–3.875722	2.402224
C	–0.153733	–5.017055	2.944534
C	1.127083	–4.897493	3.416279
C	4.202686	5.247570	–1.279340
C	3.446677	5.186349	–2.426461
C	2.912120	3.940539	–2.876346
C	1.547038	3.820422	–3.366467
C	0.946949	2.533250	–3.348575
C	–0.429095	2.405290	–2.967609
C	–0.902934	1.111602	–2.567349
C	–1.837010	1.017068	–1.498145
C	–2.056883	–0.231446	–0.883532
C	–2.534901	–0.283767	0.577710
C	–1.906284	–1.506598	1.240231
C	–1.047292	–1.412356	2.335576
C	–0.363051	–2.597432	2.788677
C	0.975938	–2.473976	3.290532
C	1.798022	–3.630941	3.385486
C	3.192904	–3.503908	3.028544
C	3.996356	–4.633354	2.664951
C	4.882199	–4.547873	1.619276
C	0.664976	4.935955	–3.447668
C	–0.663253	4.809409	–3.096433
C	–1.181794	3.562433	–2.646032
C	–2.141032	3.470694	–1.548455
C	–2.282995	2.246059	–0.874541
C	–2.403372	2.240177	0.569381
C	–2.130895	1.023650	1.255962
C	–1.268075	1.069252	2.351461
C	–0.589824	–0.123816	2.791703
C	0.732544	–0.008808	3.262362

(CC) 2018 SCS.

C	1.568563	–1.174939	3.314575
C	2.939000	–1.048664	2.984445
C	3.667076	–2.228454	2.621495
C	4.599451	–2.138813	1.532350
C	5.021278	–3.328742	0.881895
C	5.114328	–3.311840	–0.565190
C	5.073736	–4.511797	–1.341814
C	4.317376	–4.570660	–2.488844
C	–2.580727	4.652555	–0.853422
C	–2.646345	4.658577	0.513113
C	–2.306690	3.478467	1.258107
C	–1.496024	3.530592	2.448365
C	–0.803398	2.351236	2.818906
C	0.536565	2.460187	3.320796
C	1.349415	1.285937	3.329858
C	2.720212	1.407935	2.999639
C	3.448950	0.237066	2.627659
C	4.373580	0.326173	1.549914
C	4.752691	–0.874126	0.876195
C	4.849494	–0.855254	–0.540308
C	4.783697	–2.106532	–1.239594
C	3.994756	–2.169358	–2.437422
C	3.569289	–3.433780	–2.922601
C	2.204007	–3.551172	–3.412001
C	1.532550	–4.803785	–3.508963
C	0.203292	–4.918362	–3.157407
C	–1.024595	4.768106	3.003992
C	0.257626	4.870755	3.475653
C	1.141554	3.742919	3.430656
C	2.536382	3.868690	3.074124
C	3.228070	2.702189	2.652217
C	4.161043	2.792335	1.563662
C	4.534222	1.582872	0.891763
C	4.630987	1.599118	–0.524782
C	4.574121	0.361538	–1.230203
C	3.783726	0.298829	–2.423634
C	3.324218	–0.975322	–2.865492
C	1.990275	–1.090058	–3.342155
C	1.385672	–2.390701	–3.378260
C	0.009260	–2.512937	–2.997057
C	–0.526992	–3.788613	–2.691131
C	–1.486555	–3.881451	–1.593844
C	–1.708348	–5.131069	–0.914145
C	–1.770009	–5.165373	0.452139
H	–2.822358	5.595905	1.030064
H	–2.714935	5.583427	–1.393279
H	–1.266833	5.707648	–3.025755

(CC) 2018 SCS.

H	1.059791	5.928858	–3.633812
H	3.133884	6.113592	–2.894694
H	4.462904	6.220275	–0.876043
H	4.329373	6.192996	1.341741
H	2.769400	6.041680	3.185560
H	0.636944	5.846569	3.759594
H	–1.632180	5.663233	2.925257
H	1.672577	–5.794442	3.689562
H	–0.594270	–6.004232	2.855023
H	–1.775288	–6.125245	0.957668
H	–1.675074	–6.064323	–1.465328
H	–0.232194	–5.909989	–3.100481
H	2.095480	–5.708986	–3.709314
H	4.173419	–5.532514	–2.969445
H	5.503311	–5.428067	–0.951392
H	5.363794	–5.453647	1.266495
H	3.804521	–5.603309	3.110816
C	–4.084834	–0.416325	0.753322
O	–4.539811	–0.525881	1.902575
C	–6.269190	–0.529379	–0.437918
C	–6.610676	–1.782796	–1.260926
C	–6.973342	0.776910	–0.919610
O	–5.872548	–2.831368	–0.865415
N	–4.818414	–0.381951	–0.371126
S	–8.827783	0.445844	–0.870876
O	–7.447468	–1.845031	–2.136474
C	–6.558617	1.175762	–2.343916
C	–6.650788	1.912212	0.064130
H	–6.611217	–0.741533	0.578310
H	–6.141964	–3.600911	–1.397722
H	–5.914299	–0.604772	2.655348
H	–4.298949	–0.326083	–1.239875
H	–9.146458	1.511613	–0.111038
H	–7.075481	2.092484	–2.637126
H	–6.799695	0.395759	–3.067506
H	–5.481786	1.377899	–2.385727
H	–7.172796	2.825739	–0.232331
H	–5.578035	2.126316	0.055176
H	–6.943247	1.659145	1.086978
Cl	–7.017265	–0.674909	3.436885

E = –4814.963478, H = –4814.902455, G = –4815.049814 a.u.

(CC) 2018 SCS.

NTCOCl/PCA2R

C	2.950745	5.853298	1.318129
C	3.129215	5.990446	–0.036540
C	3.326457	4.839372	–0.864110
C	2.663946	4.691217	–2.145939
C	2.528240	3.381684	–2.678227
C	1.285349	2.999954	–3.287279
C	1.009768	1.599693	–3.434762
C	–0.304132	1.140897	–3.146023
C	–0.503258	–0.239974	–2.875246
C	–1.397824	–0.600852	–1.811722
C	–1.285170	–1.890165	–1.230715
C	–1.491979	–2.034217	0.168717
C	–1.043993	–3.258037	0.797909
C	–0.405337	–3.131785	2.090762
C	0.494936	–4.150409	2.500920
C	1.746473	–3.750418	3.093768
C	2.867492	–4.641793	3.196250
C	4.134380	–4.193626	2.928196
C	1.774022	5.686169	–2.658184
C	0.583687	5.319064	–3.241145
C	0.224406	3.941106	–3.349154
C	–1.121404	3.471141	–3.055892
C	–1.287875	2.098789	–2.729677
C	–2.198730	1.730179	–1.685944
C	–2.065950	0.427515	–1.099694
C	–2.270634	0.274315	0.300618
C	–1.832465	–0.903157	0.935437
C	–1.461917	–0.858914	2.418213
C	–0.311282	–1.832793	2.665129
C	0.929543	–1.415914	3.154669
C	2.016813	–2.361732	3.178989
C	3.346340	–1.893954	2.907268
C	4.359312	–2.828168	2.554737
C	5.297391	–2.454794	1.520356
C	6.055764	–3.424850	0.787946
C	6.236032	–3.286992	–0.566339
C	–2.169157	4.352843	–2.663332
C	–3.055859	3.992164	–1.669849
C	–2.944848	2.732146	–1.016558
C	–3.154034	2.581652	0.420937
C	–2.625020	1.451173	1.066623
C	–1.988459	1.607501	2.356582
C	–1.111643	0.576354	2.796072
C	0.143079	0.941072	3.284428
C	1.220720	–0.014193	3.310275
C	2.523372	0.438624	3.018724

(CC) 2018 SCS.

C	3.527802	–0.506348	2.622142
C	4.458945	–0.135252	1.622452
C	5.166379	–1.170331	0.928432
C	5.361304	–1.024448	–0.487148
C	5.674979	–2.170481	–1.264644
C	5.014780	–2.319203	–2.547497
C	4.885292	–3.589840	–3.190089
C	3.694634	–3.954217	–3.773881
C	–3.454991	3.722913	1.244190
C	–2.817779	3.890244	2.443688
C	–1.868764	2.914061	2.899046
C	–0.608873	3.288417	3.492016
C	0.444011	2.341293	3.445324
C	1.778163	2.795751	3.175317
C	2.745499	1.832194	2.755686
C	3.677740	2.199560	1.756061
C	4.380140	1.172750	1.054586
C	4.572294	1.317403	–0.348347
C	4.841222	0.149468	–1.123676
C	4.199175	0.007415	–2.382359
C	4.101330	–1.307915	–2.947555
C	2.858792	–1.689779	–3.557346
C	2.575561	–3.067028	–3.752221
C	1.229093	–3.533963	–3.457130
C	0.938208	–4.902814	–3.191045
C	0.049551	–5.251969	–2.195309
C	–0.245543	4.657825	3.724843
C	1.027051	5.090382	3.458005
C	2.014441	4.180654	2.955668
C	2.952713	4.553728	1.921235
C	3.598382	3.516771	1.196647
C	3.791578	3.662739	–0.219280
C	4.058838	2.484620	–0.990116
C	3.416922	2.340022	–2.248528
C	3.320155	1.039339	–2.823749
C	2.078390	0.657685	–3.429038
C	1.791575	–0.730678	–3.568793
C	0.476975	–1.186689	–3.279331
C	0.282678	–2.580054	–2.997199
C	–0.628324	–2.942675	–1.951863
C	–0.597101	–4.253144	–1.413438
C	–0.807278	–4.405850	0.023544
C	–0.337261	–5.576554	0.717030
C	0.309327	–5.448615	1.915782
H	–2.931632	4.828192	2.976650
H	–4.067777	4.528552	0.855131
H	–3.742662	4.742343	–1.293440

(CC) 2018 SCS.

H	–2.185947	5.374365	–3.027544
H	–0.142308	6.090808	–3.473623
H	1.950803	6.735367	–2.447510
H	2.972001	6.963923	–0.488584
H	2.659548	6.721874	1.898822
H	1.241431	6.152761	3.503773
H	–1.009286	5.385589	3.976577
H	4.944830	–4.912468	2.871956
H	2.703193	–5.703376	3.346052
H	0.797351	–6.315089	2.349099
H	–0.357029	–6.543948	0.227611
H	–0.033881	–6.297764	–1.920515
H	1.526317	–5.684893	–3.658872
H	3.570777	–4.978444	–4.109076
H	5.664111	–4.336942	–3.081876
H	6.679849	–4.106986	–1.120787
H	6.364100	–4.348124	1.266399
C	–2.591185	–1.297177	3.419707
O	–2.573658	–1.156815	4.596242
C	–7.403652	–1.035007	–1.543081
C	–6.538269	–1.483539	–0.365290
C	–8.821418	–0.525611	–1.096979
O	–5.489044	–0.673598	–0.154848
N	–7.395061	–2.152796	–2.488965
S	–8.622823	0.792178	0.221945
O	–6.742106	–2.491219	0.286163
C	–9.677192	–1.625726	–0.451209
C	–9.551832	0.076940	–2.305844
H	–6.895127	–0.192402	–2.021588
H	–4.978177	–1.034393	0.595980
H	–7.918743	–1.919000	–3.327427
H	–7.831343	–2.969171	–2.067995
H	–7.929850	1.678604	–0.521520
H	–10.653603	–1.226629	–0.162915
H	–9.194368	–2.056152	0.427715
H	–9.850598	–2.429721	–1.173126
H	–10.522191	0.477856	–2.003514
H	–9.732581	–0.689039	–3.068412
H	–8.972992	0.884642	–2.764575
Cl	–4.054173	–2.154467	2.654110

E = –4814.9290150, H = –4814.867254, G = –4815.017653 a.u.

(CC) 2018 SCS.

TS_{k5}

C	4.873260	–4.008736	–2.551223
C	5.671597	–3.802914	–1.453558
C	5.573797	–2.591360	–0.699492
C	5.576611	–2.585479	0.751172
C	5.020470	–1.459631	1.413442
C	4.186154	–1.664625	2.563159
C	3.313419	–0.598088	2.961376
C	1.991428	–0.927390	3.365135
C	0.999688	0.090518	3.360086
C	–0.313113	–0.241521	2.881658
C	–1.166845	0.805184	2.449373
C	–2.012259	0.583626	1.327780
C	–2.593823	1.739105	0.683334
C	–2.626657	1.737460	–0.758973
C	–2.696755	2.980150	–1.438785
C	–1.838991	3.176330	–2.580246
C	–1.542020	4.479108	–3.102602
C	–0.269185	4.791291	–3.502407
C	5.677980	–3.789130	1.514492
C	4.877456	–3.984170	2.615135
C	3.938478	–2.986572	3.015838
C	2.585847	–3.323586	3.433384
C	1.597249	–2.306783	3.361272
C	0.279245	–2.636775	2.906193
C	–0.572167	–1.570965	2.461183
C	–1.420669	–1.785710	1.340521
C	–2.004702	–0.676753	0.700226
C	–2.309853	–0.764084	–0.785123
C	–2.123775	0.591668	–1.439721
C	–1.225861	0.782485	–2.498536
C	–0.948509	2.128706	–2.926657
C	0.381249	2.456554	–3.354319
C	0.779917	3.819716	–3.419898
C	2.114988	4.158620	–2.981435
C	2.478321	5.486491	–2.588057
C	3.277824	5.692010	–1.491118
C	2.115971	–4.666855	3.485016
C	0.843473	–4.982472	3.058369
C	–0.028593	–3.975167	2.558194
C	–0.892433	–4.198301	1.404077
C	–1.385334	–3.083994	0.706552
C	–1.401066	–3.109741	–0.735170
C	–1.493473	–1.867963	–1.425879
C	–0.614658	–1.621626	–2.484409
C	–0.349785	–0.276645	–2.916427
C	0.964888	0.052823	–3.313014

(CC) 2018 SCS.

C	1.371036	1.427127	–3.332733
C	2.684595	1.758167	–2.918991
C	2.958488	3.109585	–2.528796
C	3.798901	3.326281	–1.384862
C	3.765715	4.584643	–0.728349
C	3.770788	4.592228	0.721988
C	3.291797	5.707084	1.476647
C	2.493671	5.509158	2.578468
C	–0.877453	–5.452118	0.701732
C	–0.855489	–5.473571	–0.665614
C	–0.874601	–4.244253	–1.404331
C	–0.022811	–4.020807	–2.546907
C	0.266092	–2.680214	–2.904804
C	1.591862	–2.341886	–3.335615
C	1.974401	–0.965452	–3.322974
C	3.286672	–0.631317	–2.909396
C	3.566491	0.711562	–2.514358
C	4.398641	0.925675	–1.377924
C	4.318752	2.179162	–0.701132
C	4.328678	2.186168	0.718878
C	3.813424	3.342452	1.394332
C	2.980273	3.137500	2.544907
C	2.136897	4.189081	2.988471
C	0.784352	3.849807	3.403925
C	–0.264634	4.812303	3.444222
C	–1.533431	4.486143	3.014830
C	0.857478	–5.032045	–3.056948
C	2.126107	–4.707176	–3.460051
C	2.588821	–3.353384	–3.391521
C	3.924754	–3.014912	–2.953996
C	4.168474	–1.688376	–2.510215
C	5.008589	–1.472472	–1.365755
C	4.920814	–0.211013	–0.691473
C	4.929336	–0.202052	0.728444
C	4.426644	0.943909	1.409984
C	3.591226	0.738400	2.556315
C	2.714321	1.787973	2.952420
C	1.392872	1.456294	3.355825
C	0.394053	2.486001	3.341603
C	–0.921621	2.150573	2.883473
C	–1.824032	3.182102	2.524135
C	–2.687908	2.960700	1.369713
C	–3.268867	4.065963	0.656485
C	–3.261100	4.079656	–0.710628
H	–0.688471	–6.414383	–1.179295
H	–0.737133	–6.378287	1.248234
H	0.570441	–6.028598	2.970631

(CC) 2018 SCS.

H	2.803726	–5.474690	3.712043
H	4.858767	–4.964651	3.079498
H	6.266529	–4.620878	1.141773
H	6.268857	–4.627718	–1.078887
H	4.862485	–4.989145	–3.015611
H	2.820020	–5.504689	–3.704937
H	0.574145	–6.077129	–2.992163
H	–0.035916	5.819886	–3.757540
H	–2.288360	5.264542	–3.049981
H	–3.561576	4.980662	–1.234701
H	–3.583116	4.953948	1.193989
H	–2.267880	5.278522	2.917545
H	–0.040981	5.850826	3.664455
H	2.013894	6.367954	3.036341
H	3.417885	6.715278	1.096188
H	3.411806	6.704174	–1.123782
H	2.004090	6.341011	–3.059127
C	–3.804899	–1.138128	–1.193589
O	–4.441272	–1.457368	–2.092510
C	–7.279339	0.042258	0.922000
C	–6.083739	0.441182	0.043479
C	–8.470330	–0.555644	0.091711
O	–4.942172	–0.268282	0.265405
N	–7.581781	1.233384	1.717228
S	–7.835673	–1.889095	–1.053476
O	–6.090883	1.371253	–0.727926
C	–9.136090	0.487865	–0.817795
C	–9.501445	–1.158811	1.058383
H	–6.951012	–0.740535	1.613506
H	–5.052830	–1.196587	0.758995
H	–8.361057	1.059784	2.344545
H	–7.828684	2.004136	1.102508
H	–7.071507	–2.558258	–0.152062
H	–9.929038	0.021535	–1.410239
H	–8.413890	0.949673	–1.493102
H	–9.598020	1.275737	–0.212715
H	–10.330968	–1.599890	0.500264
H	–9.917939	–0.388870	1.721452
H	–9.055173	–1.941875	1.678662
Cl	–4.905724	–2.936680	1.106917

E = –4814.895086, H = –4814.834121, G = –4814.979940 a.u.

(CC) 2018 SCS.

NTCOO/HClP

C	–4.475496	–4.523599	2.271327
C	–5.287203	–4.333766	1.180063
C	–5.300617	–3.077681	0.493778
C	–5.301317	–2.991992	–0.954227
C	–4.853152	–1.783194	–1.549829
C	–3.996702	–1.846015	–2.700323
C	–3.227188	–0.680964	–3.031154
C	–1.876060	–0.862136	–3.433445
C	–0.986011	0.243337	–3.361635
C	0.347485	0.011132	–2.881345
C	1.093792	1.108153	–2.380396
C	1.951497	0.905084	–1.264000
C	2.432744	2.074537	–0.557286
C	2.470485	1.995263	0.887548
C	2.410787	3.203805	1.629561
C	1.534712	3.254568	2.772830
C	1.110173	4.493944	3.360196
C	–0.190810	4.661582	3.756535
C	–5.287088	–4.157348	–1.782329
C	–4.465498	–4.216318	–2.883882
C	–3.622214	–3.113338	–3.218776
C	–2.238924	–3.298497	–3.632659
C	–1.353095	–2.196858	–3.495030
C	–0.012808	–2.425176	–3.040562
C	0.728322	–1.308303	–2.528461
C	1.590702	–1.502218	–1.412209
C	2.056542	–0.380676	–0.704393
C	2.436100	–0.537176	0.779835
C	2.089001000	0.768234	1.501562
C	1.159066	0.819451	2.544760
C	0.747248	2.107971	3.044010
C	–0.612923	2.284869	3.466828
C	–1.140259	3.599311	3.601561
C	–2.498786	3.834067	3.167748
C	–2.985373	5.142611	2.845986
C	–3.799071	5.332952	1.756232
C	–1.642959	–4.586614	–3.750161
C	–0.346837	–4.803152	–3.329095
C	0.422550	–3.745759	–2.766695
C	1.304485	–3.950692	–1.619863
C	1.689401	–2.836894	–0.855021
C	1.708368	–2.943648	0.588317
C	1.691948	–1.739325	1.346255
C	0.774849	–1.636197	2.391002
C	0.377356	–0.341721	2.885082
C	–0.963124	–0.159004	3.279502

(CC) 2018 SCS.

C	–1.498794	1.169144	3.371396
C	–2.835673	1.396992	2.965602
C	–3.235942	2.736198	2.649716
C	–4.092308	2.936111	1.514151
C	–4.177239	4.227380	0.929365
C	–4.180962	4.314970	–0.518343
C	–3.806220	5.511224	–1.205928
C	–2.987672	5.450241	–2.309322
C	1.401095	–5.241345	–0.989745
C	1.372675	–5.341365	0.374507
C	1.276798	–4.158413	1.182344
C	0.402503	–4.080350	2.326086
C	–0.010525	–2.792103	2.745910
C	–1.366498	–2.601363	3.174446
C	–1.874351	–1.267312	3.225654
C	–3.210529	–1.035576	2.821193
C	–3.613631	0.295464	2.496073
C	–4.462469	0.493052	1.371036
C	–4.500853	1.784802	0.764907
C	–4.510594	1.869551	–0.652428
C	–4.104863	3.105387	–1.258678
C	–3.250241	3.043166	–2.410597
C	–2.506927	4.192675	–2.785979
C	–1.124326	4.004557	–3.200148
C	–0.170554	5.061936	–3.174401
C	1.121835	4.833172	–2.748299
C	–0.384573	–5.196283	2.769887
C	–1.681223	–5.012136	3.172963
C	–2.265607	–3.703339	3.166162
C	–3.625075	–3.467681	2.734521
C	–3.989450	–2.147031	2.360567
C	–4.844363	–1.948075	1.223464
C	–4.874957	–0.648615	0.619925
C	–4.883160	–0.561640	–0.797272
C	–4.489326	0.663054	–1.411406
C	–3.633238	0.600209	–2.559046
C	–2.856454	1.748194	–2.887560
C	–1.505838	1.564212	–3.290042
C	–0.608877	2.681160	–3.205917
C	0.728566	2.446786	–2.746970
C	1.530035	3.536729	–2.325586
C	2.410421	3.333745	–1.177389
C	2.879697	4.452945	–0.402294
C	2.864831	4.393064	0.964013
H	1.283998	–6.321160	0.831663
H	1.342773	–6.144512	–1.587068
H	0.021418	–5.822655	–3.294998

(CC) 2018 SCS.

H	–2.248469	–5.443290	–4.025677
H	–4.351947	–5.164265	–3.399027
H	–5.795772	–5.059871	–1.460986
H	–5.803128	–5.189168	0.757095
H	–4.374739	–5.522646	2.681504
H	–2.299906	–5.881659	3.367707
H	–0.005119	–6.205972	2.655315
H	–0.524001	5.647191	4.063673
H	1.777903	5.348731	3.362118
H	3.067215	5.292311	1.535997
H	3.103607	5.396252	–0.887972
H	1.775005	5.685950	–2.598698
H	–0.489230	6.085841	–3.337446
H	–2.588062	6.374277	–2.713463
H	–4.027117	6.480405	–0.771778
H	–4.028262	6.346833	1.445955
H	–2.596617	6.010620	3.367442
C	3.956849	–0.766084	1.001385
O	4.415825	–1.510032	1.835788
C	6.631971	1.007210	–0.868940
C	6.029354	0.346478	0.369441
C	7.777130	0.140710	–1.503582
O	4.702976	–0.017396	0.129325
N	6.989706	2.363849	–0.456676
S	7.125752	–1.593385	–1.792176
O	6.563796	0.236439	1.439482
C	8.991295	–0.025269	–0.577695
C	8.205523	0.764215	–2.838725
H	5.836738	1.090139	–1.614423
H	6.070891	–2.120955	2.373454
H	7.281813	2.915343	–1.257786
H	7.757934	2.348163	0.208960
H	6.154139	–1.269712	–2.669716
H	9.760348	–0.625646	–1.070972
H	8.728917	–0.500524	0.369371
H	9.428993	0.953848	–0.360275
H	8.969405	0.147712	–3.318233
H	8.633569	1.759191	–2.674139
H	7.361089	0.865541	–3.527323
Cl	7.052216	–2.825961	2.881619

E = –4814.873667, H = –4814.935269, G = –4815.022033 a.u.

(CC) 2018 SCS.

NTCOCl/PCA3R

C	3.127987	5.025360	3.013777
C	4.146800	5.086079	2.095049
C	4.554899	3.912808	1.383864
C	4.837145	3.935098	–0.038859
C	4.775950	2.706929	–0.749220
C	4.152032	2.676883	–2.041871
C	3.725828	1.406463	–2.554670
C	2.465994	1.335924	–3.208947
C	1.837043	0.069248	–3.349060
C	0.419918	–0.012246	–3.130997
C	–0.151901	–1.272922	–2.821608
C	–1.219234	–1.331958	–1.884452
C	–1.557925	–2.622485	–1.323345
C	–1.875622	–2.658001	0.087915
C	–1.697017	–3.879922	0.788661
C	–1.054820	–3.833653	2.078319
C	–0.489115	–4.999711	2.696096
C	0.721319	–4.926101	3.334186
C	4.723257	5.130284	–0.815097
C	4.124493	5.100025	–2.053013
C	3.615786	3.875007	–2.582452
C	2.326612	3.802516	–3.254433
C	1.688528	2.535771	–3.329681
C	0.269963	2.451054	–3.139448
C	–0.295099	1.171749	–2.817959
C	–1.366689	1.102716	–1.883355
C	–1.703575	–0.139417	–1.314807
C	–2.357802	–0.174485	0.068554
C	–1.880567	–1.426988	0.803328
C	–1.173770	–1.363157	2.008180
C	–0.595317	–2.573345	2.536203
C	0.668795	–2.498642	3.212343
C	1.431983	–3.683455	3.404616
C	2.865517	–3.603057	3.236315
C	3.671365	–4.757523	2.971105
C	4.691805	–4.696654	2.054203
C	1.499818	4.946496	–3.446192
C	0.132709	4.861968	–3.279943
C	–0.481404	3.631069	–2.912372
C	–1.578931	3.566655	–1.950839
C	–1.848182	2.343938	–1.312698
C	–2.151187	2.338584	0.102397
C	–2.009870	1.111622	0.809115
C	–1.304558	1.121656	2.012199
C	–0.737930	–0.095457	2.534315
C	0.514635	–0.028063	3.177661

(CC) 2018 SCS.

C	1.296652	–1.221367	3.329597
C	2.702850	–1.140508	3.185206
C	3.432445	–2.342557	2.908879
C	4.503688	–2.279072	1.954091
C	4.968838	–3.479220	1.354203
C	5.254896	–3.458020	–0.067652
C	5.278863	–4.651913	–0.853956
C	4.683239	–4.679209	–2.093220
C	–2.064734	4.759640	–1.308775
C	–2.308564	4.762794	0.037777
C	–2.108697	3.569015	0.809471
C	–1.462991	3.588308	2.098493
C	–0.866600	2.385133	2.550029
C	0.395167	2.445683	3.230741
C	1.159869	1.244136	3.338900
C	2.565881	1.321185	3.195712
C	3.298493	0.128422	2.912338
C	4.359598	0.191849	1.965582
C	4.784330	–1.016836	1.336197
C	5.069466	–0.993976	–0.054765
C	5.056539	–2.238764	–0.768547
C	4.434681	–2.268906	–2.062146
C	4.038900	–3.515680	–2.613338
C	2.749523	–3.585260	–3.284730
C	2.057807	–4.814947	–3.481337
C	0.690873	–4.887616	–3.308471
C	–1.031398	4.806113	2.724953
C	0.177063	4.862804	3.368748
C	1.021258	3.706189	3.434110
C	2.455233	3.786431	3.268803
C	3.157881	2.599418	2.930904
C	4.227933	2.663577	1.974614
C	4.646320	1.445561	1.346041
C	4.930386	1.465914	–0.045143
C	4.927526	0.234770	–0.763585
C	4.303034	0.204587	–2.053080
C	3.866443	–1.051024	–2.564936
C	2.606602	–1.118734	–3.219154
C	1.971382	–2.398875	–3.349203
C	0.553802	–2.477646	–3.153322
C	–0.057190	–3.736649	–2.930962
C	–1.153108	–3.802650	–1.967794
C	–1.505380	–5.046858	–1.335222
C	–1.755833	–5.084790	0.009176
H	–2.519315	5.703609	0.534903
H	–2.094275	5.697156	–1.852880
H	–0.446199	5.779033	–3.287049

(CC) 2018 SCS.

H	1.947357	5.926460	–3.571793
H	3.905458	6.039856	–2.548584
H	4.957883	6.091861	–0.371435
H	4.534786	6.057696	1.808376
H	2.741301	5.949661	3.429203
H	0.545535	5.824159	3.710454
H	–1.591928	5.722064	2.572098
H	1.196699	–5.842547	3.667147
H	–0.945222	–5.971044	2.538558
H	–1.862255	–6.046017	0.500573
H	–1.427435	–5.978238	–1.885025
H	0.219954	–5.864550	–3.317975
H	2.613566	–5.737002	–3.613448
H	4.573993	–5.633188	–2.597911
H	5.620956	–5.584349	–0.418009
H	5.185087	–5.616799	1.759855
H	3.388880	–5.722843	3.377102
C	–3.925761	–0.263303	0.070485
O	–4.634378	0.016477	0.983348
C	–8.378183	0.670925	0.404561
C	–9.000319	1.160452	–0.902400
C	–8.904457	–0.746148	0.832591
O	–8.109335	1.225238	–1.907923
N	–8.588236	1.751187	1.371150
S	–8.690247	–1.942152	–0.596255
O	–10.159912	1.505741	–1.024996
C	–10.405830	–0.759533	1.155801
C	–8.093443	–1.245537	2.037463
H	–7.299991	0.577666	0.246189
H	–8.580680	1.558568	–2.692661
H	–8.144437	1.530226	2.257734
H	–9.581960	1.878546	1.544630
H	–7.355449	–1.805242	–0.738293
H	–10.722803	–1.766301	1.442304
H	–11.008576	–0.423560	0.310427
H	–10.608092	–0.098312	2.004130
H	–8.407790	–2.253916	2.317303
H	–8.255563	–0.594454	2.904110
H	–7.021383	–1.261886	1.820283
Cl	–4.679725	–0.911508	–1.476035

E = –4814.928681, H = –4814.866859, G = –4815.018050 a.u.

(CC) 2018 SCS.

TS_{k6}

C	5.305087	–3.805373	–2.057746
C	5.969395	–3.539201	–0.883794
C	5.730754	–2.321650	–0.174854
C	5.579816	–2.291426	1.269707
C	4.901726	–1.185288	1.845490
C	3.965621	–1.415945	2.908410
C	3.000328	–0.392963	3.190924
C	1.662647	–0.788996	3.463154
C	0.623391	0.171231	3.333641
C	–0.611396	–0.241651	2.726567
C	–1.471529	0.747926	2.184864
C	–2.173042	0.464182	0.981947
C	–2.731977	1.574060	0.254872
C	–2.602699	1.543225	–1.176821
C	–2.684891	2.763567	–1.895257
C	–1.723125	2.994838	–2.953297
C	–1.447121	4.302614	–3.464451
C	–0.155133	4.682570	–3.736596
C	5.667535	–3.474781	2.064599
C	4.769630	–3.694795	3.083779
C	3.744605	–2.741753	3.363457
C	2.375128	–3.146455	3.645152
C	1.346766	–2.187821	3.448997
C	0.104498	–2.598824	2.864577
C	–0.751437	–1.589922	2.308962
C	–1.456402	–1.868928	1.105795
C	–2.022926	–0.802366	0.366705
C	–2.105962	–0.907652	–1.116115
C	–1.956195	0.407842	–1.760663
C	–0.984599	0.643771	–2.750996
C	–0.744219	1.995965	–3.180013
C	0.601544	2.392104	–3.477533
C	0.928411	3.773254	–3.529107
C	2.193421	4.193303	–2.957166
C	2.439400	5.543891	–2.558228
C	3.104064	5.811121	–1.384664
C	1.977054	–4.514549	3.682147
C	0.776898	–4.909217	3.130931
C	–0.087553	–3.958575	2.514669
C	–0.797931	–4.245423	1.275020
C	–1.269740	–3.162266	0.504200
C	–1.141063	–3.203281	–0.926052
C	–1.237295	–1.968628	–1.642271
C	–0.265667	–1.708840	–2.630118
C	–0.025414	–0.368255	–3.058354
C	1.313561	0.029551	–3.329138

(CC) 2018 SCS.

C	1.639879	1.418821	–3.332098
C	2.883034	1.829126	–2.786407
C	3.037903	3.199586	–2.396019
C	3.735493	3.479690	–1.173120
C	3.564314	4.744218	–0.552649
C	3.409256	4.774350	0.891954
C	2.792486	5.873463	1.563426
C	1.893604	5.650653	2.581209
C	–0.643254	–5.501239	0.601518
C	–0.486407	–5.534428	–0.760378
C	–0.500046	–4.320008	–1.518963
C	0.451165	–4.074156	–2.581111
C	0.705129	–2.725872	–2.935928
C	2.050824	–2.326224	–3.230984
C	2.362162	–0.930616	–3.209665
C	3.604915	–0.519930	–2.662287
C	3.769245	0.839861	–2.270703
C	4.459035	1.116880	–1.048176
C	4.239164	2.372882	–0.412686
C	4.094697	2.403416	1.000717
C	3.448854	3.540316	1.592267
C	2.511012	3.309035	2.653620
C	1.571416	4.319866	2.984030
C	0.202132	3.911790	3.265413
C	–0.895335	4.817256	3.181026
C	–2.094389	4.414849	2.632894
C	1.425167	–5.044638	–2.979038
C	2.715280	–4.659455	–3.251697
C	3.096901	–3.284667	–3.159298
C	4.360668	–2.868573	–2.582135
C	4.487589	–1.523660	–2.144699
C	5.184114	–1.245231	–0.920797
C	4.960456	0.021726	–0.287265
C	4.816439	0.053669	1.126290
C	4.186970	1.181366	1.725756
C	3.244901	0.948652	2.784176
C	2.277342	1.954302	3.063892
C	0.940479	1.556245	3.336751
C	–0.105270	2.527997	3.196351
C	–1.346872	2.111962	2.613241
C	–2.259984	3.087738	2.141248
C	–2.975259	2.803714	0.902949
C	–3.534042	3.855186	0.105305
C	–3.381263	3.839777	–1.258288
H	–0.212455	–6.469797	–1.236237
H	–0.499491	–6.412560	1.171046
H	0.572328	–5.970433	3.040955

(CC) 2018 SCS.

H	2.678780	–5.278110	3.999499
H	4.754396	–4.667073	3.564259
H	6.332635	–4.279766	1.771745
H	6.560426	–4.326536	–0.428821
H	5.392745	–4.793538	–2.495992
H	3.468658	–5.424227	–3.406331
H	1.192063	–6.102302	–2.923516
H	0.044766	5.720659	–3.979244
H	–2.232812	5.049321	–3.498019
H	–3.667074	4.716586	–1.829132
H	–3.943279	4.740635	0.578873
H	–2.855464	5.164141	2.444940
H	–0.751430	5.869430	3.400408
H	1.322055	6.489229	2.964000
H	2.900891	6.879701	1.173751
H	3.140937	6.834441	–1.027121
H	1.973767	6.363612	–3.094248
C	–3.861725	–1.413113	–1.793832
O	–4.109864	–1.534740	–2.917671
C	–8.053630	–0.862788	0.921894
C	–7.762132	0.317870	1.846760
C	–7.408996	–0.701321	–0.504400
O	–6.893386	0.015240	2.826144
N	–9.504119	–1.035718	0.955520
S	–5.557810	–0.555627	–0.199147
O	–8.296367	1.405959	1.748847
C	–7.822717	0.582476	–1.233016
C	–7.744730	–1.943714	–1.338931
H	–7.579506	–1.750551	1.350217
H	–6.775707	0.815518	3.369166
H	–9.792945	–1.819711	0.379215
H	–9.963992	–0.198383	0.607525
H	–5.293760	–1.848279	0.184076
H	–7.425206	0.582328	–2.251460
H	–7.479031	1.481398	–0.718116
H	–8.914544	0.631801	–1.303381
H	–7.206605	–1.937864	–2.289052
H	–8.816816	–1.947204	–1.564106
H	–7.492067	–2.862678	–0.804003
Cl	–4.638893	–3.792774	–0.558379

E = –4814.898620, H = –4814.839243, G =4814.980056 a.u.

(CC) 2018 SCS.

NTCOS/HClP

C	–3.934620	–4.707209	2.586152
C	–4.823926	–4.615197	1.543963
C	–4.976042	–3.387172	0.824131
C	–5.074053	–3.350598	–0.622156
C	–4.756930	–2.132799	–1.280374
C	–3.972583	–2.171129	–2.482527
C	–3.314907	–0.964832	–2.896244
C	–1.982151	–1.060467	–3.380408
C	–1.174338	0.108833	–3.399120
C	0.200365	–0.009203	–3.001575
C	0.895548	1.155470	–2.586855
C	1.835801	1.054075	–1.523910
C	2.268216	2.279307	–0.883382
C	2.388361	2.255231	0.559445
C	2.284022	3.482023	1.266923
C	1.478376	3.509752	2.461745
C	0.998663	4.734826	3.037632
C	–0.281827	4.819038	3.517638
C	–5.025454	–4.538848	–1.416142
C	–4.273662	–4.574258	–2.567165
C	–3.537660	–3.424485	–2.987717
C	–2.173788	–3.522171	–3.485415
C	–1.365952	–2.354895	–3.437746
C	0.013167	–2.469565	–3.064330
C	0.699973	–1.284933	–2.634975
C	1.641576	–1.376295	–1.572293
C	2.073901	–0.200105	–0.929916
C	2.541350	–0.266377	0.531394
C	2.127116	1.026547	1.228046
C	1.271941	1.048409	2.330726
C	0.798921	2.318985	2.819803
C	–0.539198	2.408488	3.330219
C	–1.155650	3.683767	3.461344
C	–2.552908	3.801373	3.112084
C	–3.157556	5.058504	2.784358
C	–4.047376	5.150491	1.742761
C	–1.491372	–4.766946	–3.604422
C	–0.159482	–4.874259	–3.260354
C	0.561828	–3.744770	–2.779637
C	1.525356	–3.844200	–1.686160
C	1.872240	–2.678809	–0.982887
C	1.991431	–2.731127	0.459307
C	1.926460	–1.504663	1.178110
C	1.075300	–1.434305	2.281749
C	0.608229	–0.156665	2.758752
C	–0.712392	–0.061068	3.238452

(CC) 2018 SCS.

C	–1.341124	1.226655	3.326801
C	–2.714190	1.340363	3.003161
C	–3.235034	2.634585	2.675545
C	–4.171520	2.731466	1.590570
C	–4.388768	3.992118	0.973904
C	–4.484268	4.029604	–0.472638
C	–4.242381	5.226098	–1.217131
C	–3.490749	5.188220	–2.368232
C	1.759877	–5.101101	–1.023997
C	1.826080	–5.154101	0.341315
C	1.691007	–3.953180	1.117344
C	0.888462	–3.900329	2.312812
C	0.405270	–2.632428	2.721028
C	–0.932357	–2.528721	3.231648
C	–1.536944	–1.235757	3.277249
C	–2.909736	–1.117709	2.953490
C	–3.432942	0.168080	2.616579
C	–4.361158	0.263888	1.542490
C	–4.534748	1.528159	0.902380
C	–4.635761	1.563570	–0.513525
C	–4.361979	2.804357	–1.180247
C	–3.577177	2.766398	–2.382135
C	–2.947342	3.953883	–2.838699
C	–1.583577	3.853118	–3.337792
C	–0.711854	4.977354	–3.408507
C	0.619144	4.857811	–3.065049
C	0.219448	–5.055759	2.842450
C	–1.059826	–4.955130	3.322335
C	–1.743161	–3.694620	3.313385
C	–3.140434	–3.575680	2.963342
C	–3.627678	–2.299012	2.575728
C	–4.563656	–2.202629	1.490338
C	–4.730325	–0.930234	0.852613
C	–4.831791	–0.892203	–0.563199
C	–4.569970	0.336701	–1.236609
C	–3.784675	0.298461	–2.434718
C	–3.118424	1.488490	–2.846464
C	–1.786056	1.390004	–3.331387
C	–0.971702	2.571381	–3.339766
C	0.407211	2.450424	–2.966775
C	1.150549	3.609824	–2.632832
C	2.113336	3.511761	–1.538791
C	2.541428	4.688178	–0.827795
C	2.610472	4.676019	0.538399
H	1.842356	–6.120651	0.833727
H	1.734345	–6.026730	–1.588345
H	0.285713	–5.862444	–3.220392

(CC) 2018 SCS.

H	–2.046832	–5.674211	–3.816153
H	–4.123344	–5.527670	–3.062457
H	–5.445393	–5.464499	–1.037442
H	–5.297845	–5.520370	1.179419
H	–3.732435	–5.681578	3.017661
H	–1.595154	–5.861036	3.586143
H	0.668736	–6.037348	2.736337
H	–0.668576	5.787243	3.817238
H	1.597899	5.636353	2.968606
H	2.778722	5.607554	1.068281
H	2.664115	5.628003	–1.354890
H	1.215099	5.760379	–2.984791
H	–1.116241	5.969025	–3.580302
H	–3.188067	6.124975	–2.824059
H	–4.508759	6.190618	–0.798436
H	–4.372589	6.133105	1.417876
H	–2.805972	5.970178	3.255182
C	4.097769	–0.392651	0.740942
O	4.550133	–0.435789	1.869866
C	7.655654	–0.745574	–1.573838
C	7.596334	0.571594	–2.348640
C	6.844128	–0.680018	–0.209594
O	6.667953	0.558774	–3.320468
N	9.070997	–1.068412	–1.439273
S	5.048143	–0.444493	–0.758958
O	8.315570	1.524747	–2.125967
C	7.324018	0.466972	0.689197
C	6.965365	–2.037213	0.502705
H	7.187547	–1.518951	–2.190932
H	6.671728	1.436114	–3.744008
H	9.205765	–1.922309	–0.907593
H	9.562265	–0.314292	–0.967127
H	5.373298	–0.276717	3.471286
H	6.929175	0.364367	1.699477
H	7.053838	1.447711	0.293446
H	8.415584	0.422562	0.766662
H	6.310292	–2.077984	1.373174
H	7.989738	–2.178382	0.862180
H	6.713299	–2.864838	–0.166541
Cl	5.966697	–0.162046	4.625709

E = –4814.937351, H = –4814.876573, G = –4815.023160 a.u.

(CC) 2018 SCS.

UM062X

NTCOOH

C	4.889808	–2.134571	2.940650
C	4.888329	–3.142648	2.015587
C	3.687925	–3.485371	1.320357
C	3.688789	–3.753665	–0.106148
C	2.472198	–3.615621	–0.807038
C	2.472664	–2.978810	–2.089850
C	1.225001	–2.473808	–2.590603
C	1.223566	–1.212178	–3.231796
C	0.000001	–0.514627	–3.366959
C	0.000005	0.905919	–3.134025
C	–1.217878	1.539943	–2.806239
C	–1.212529	2.589690	–1.855332
C	–2.480261	3.006913	–1.288263
C	–2.495333	3.301808	0.129385
C	–3.715359	3.178219	0.825308
C	–3.705094	2.518420	2.104150
C	–4.905385	2.004581	2.700782
C	–4.897253	0.792514	3.326714
C	4.887057	–3.685424	–0.875726
C	4.885763	–3.075443	–2.104100
C	3.688279	–2.509529	–2.627018
C	3.687612	–1.208954	–3.285974
C	2.467893	–0.503611	–3.350373
C	2.464364	0.910756	–3.141379
C	1.217890	1.539936	–2.806236
C	1.212545	2.589683	–1.855329
C	0.000008	2.977018	–1.273590
C	0.000007	3.632514	0.104711
C	–1.265270	3.211850	0.836599
C	–1.244540	2.499669	2.026892
C	–2.481149	1.991095	2.557176
C	–2.474252	0.718686	3.220899
C	–3.690165	0.023212	3.401774
C	–3.688867	–1.409120	3.219738
C	–4.889829	–2.134545	2.940639
C	–4.888353	–3.142622	2.015576
C	4.877623	–0.451608	–3.447978
C	4.870842	0.912159	–3.262251
C	3.675385	1.588209	–2.904232
C	3.673113	2.680628	–1.930137
C	2.480278	3.006899	–1.288258
C	2.495347	3.301796	0.129390
C	1.265282	3.211844	0.836601
C	1.244544	2.499663	2.026895
C	0.000001	1.988172	2.544200

(CC) 2018 SCS.

C	–0.000003	0.737319	3.170379
C	–1.234011	0.020430	3.319715
C	–1.230335	–1.379074	3.159046
C	–2.471040	–2.039269	2.885245
C	–2.470914	–3.098569	1.917839
C	–3.687950	–3.485351	1.320348
C	–3.688812	–3.753645	–0.106156
C	–4.887078	–3.685397	–0.875737
C	–4.885778	–3.075417	–2.104111
C	4.897224	3.079403	–1.288678
C	4.919514	3.307095	0.054464
C	3.715370	3.178200	0.825316
C	3.705099	2.518402	2.104158
C	2.481150	1.991083	2.557181
C	2.474245	0.718673	3.220904
C	1.234000	0.020424	3.319718
C	1.230318	–1.379080	3.159048
C	–0.000010	–2.040712	2.875681
C	–0.000012	–3.089856	1.917970
C	–1.228370	–3.435830	1.288791
C	–1.226482	–3.703732	–0.099592
C	–2.472218	–3.615608	–0.807043
C	–2.472678	–2.978796	–2.089856
C	–3.688289	–2.509509	–2.627026
C	–3.687614	–1.208934	–3.285982
C	–4.877620	–0.451581	–3.447989
C	–4.870832	0.912186	–3.262263
C	4.905385	2.004556	2.700792
C	4.897246	0.792489	3.326724
C	3.690155	0.023193	3.401782
C	3.688849	–1.409139	3.219745
C	2.471020	–2.039282	2.885250
C	2.470891	–3.098583	1.917845
C	1.228346	–3.435837	1.288794
C	1.226460	–3.703739	–0.099589
C	–0.000010	–3.628270	–0.811111
C	–0.000007	–2.989141	–2.095101
C	–1.225011	–2.473801	–2.590606
C	–1.223568	–1.212172	–3.231799
C	–2.467890	–0.503598	–3.350378
C	–2.464354	0.910769	–3.141384
C	–3.675373	1.588229	–2.904241
C	–3.673097	2.680648	–1.930146
C	–4.897207	3.079429	–1.288690
C	–4.919500	3.307120	0.054453
H	5.871908	3.456270	0.551684
H	5.831671	3.060880	–1.838309

(CC) 2018 SCS.

H	5.820399	1.435580	–3.245538
H	5.832015	–0.953093	–3.565360
H	5.835004	–2.894009	–2.596574
H	5.836206	–3.968128	–0.433532
H	5.835219	–3.575959	1.711995
H	5.836748	–1.797094	3.347541
H	5.837348	0.361520	3.653838
H	5.850163	2.512740	2.541331
H	–5.837358	0.361550	3.653826
H	–5.850159	2.512770	2.541318
H	–5.871894	3.456300	0.551670
H	–5.831653	3.060911	–1.838323
H	–5.820386	1.435612	–3.245553
H	–5.832015	–0.953061	–3.565375
H	–5.835016	–2.893977	–2.596587
H	–5.836229	–3.968096	–0.433545
H	–5.835245	–3.575928	1.711982
H	–5.836768	–1.797063	3.347528
C	0.000022	5.176487	0.060962
O	–0.000099	5.860868	1.054665
O	0.000203	5.666024	–1.179210
H	0.000219	6.636035	–1.116804

E = –3628.884123

NTCOOH/PCA1

C	–4.722939	–3.490452	3.226754
C	–5.734728	–3.014430	2.437481
C	–5.606577	–1.753796	1.778355
C	–6.020404	–1.575854	0.398030
C	–5.455713	–0.507146	–0.329361
C	–5.040977	–0.724327	–1.682486
C	–4.110313	0.205891	–2.258706
C	–3.058187	–0.308487	–3.053072
C	–1.922326	0.500329	–3.290976
C	–0.624408	–0.120384	–3.240789
C	0.507176	0.691784	–3.010045
C	1.557140	0.193034	–2.202525
C	2.541229	1.136097	–1.706851
C	2.982890	0.959619	–0.342031
C	3.481454	2.082951	0.350563
C	3.049720	2.296640	1.706135
C	3.181731	3.571955	2.349474
C	2.169408	4.057952	3.125091
C	–6.570373	–2.650751	–0.359339
C	–6.172823	–2.857152	–1.656064
C	–5.211678	–1.998482	–2.260675
C	–4.126460	–2.529164	–3.077775

(CC) 2018 SCS.

C	–2.976322	–1.730080	–3.243712
C	–1.685802	–2.343870	–3.215705
C	–0.543951	–1.505027	–2.980019
C	0.512489	–1.994775	–2.172748
C	1.453944	–1.094038	–1.661038
C	2.203826	–1.440555	–0.375686
C	2.462288	–0.146489	0.384359
C	1.960902	0.087711	1.657405
C	2.103409	1.398669	2.234106
C	1.043608	1.910110	3.054538
C	0.969568	3.297438	3.309261
C	–0.333649	3.920848	3.307609
C	–0.494643	5.327268	3.106317
C	–1.506402	5.800971	2.315570
C	–3.983159	–3.919995	–3.321084
C	–2.738777	–4.508969	–3.309879
C	–1.575465	–3.737938	–3.052824
C	–0.480852	–4.249535	–2.226344
C	0.403541	–3.342350	–1.645238
C	0.831812	–3.544687	–0.277914
C	1.372460	–2.428069	0.417700
C	0.884193	–2.157011	1.686712
C	1.026974	–0.836929	2.249019
C	–0.015515	–0.326095	3.030166
C	–0.105222	1.087589	3.254382
C	–1.376754	1.693280	3.271958
C	–1.462538	3.108293	3.068239
C	–2.524331	3.606996	2.243719
C	–2.416450	4.897690	1.686156
C	–2.830507	5.076852	0.306008
C	–2.346894	6.162112	–0.481107
C	–1.950783	5.953612	–1.777790
C	–0.576537	–5.552603	–1.625965
C	–0.218270	–5.730085	–0.323172
C	0.279992	–4.623319	0.442494
C	–0.151651	–4.387782	1.795715
C	–0.041051	–3.076673	2.294399
C	–1.095352	–2.551524	3.113276
C	–1.171614	–1.136773	3.283686
C	–2.440067	–0.524966	3.301852
C	–2.533452	0.881096	3.090050
C	–3.586401	1.375532	2.274197
C	–3.439851	2.659406	1.679093
C	–3.848808	2.834013	0.337258
C	–3.317336	3.951237	–0.390994
C	–2.903116	3.735223	–1.744486
C	–2.023949	4.653431	–2.353196

(CC) 2018 SCS.

C	–0.940930	4.121382	–3.172522
C	0.230136	4.875755	–3.445669
C	1.469335	4.275783	–3.434977
C	–1.058150	–5.274474	2.467735
C	–2.063817	–4.772426	3.241576
C	–2.220443	–3.356786	3.397690
C	–3.522803	–2.731863	3.397334
C	–3.599398	–1.348310	3.129481
C	–4.661722	–0.849457	2.305622
C	–4.502259	0.444553	1.709851
C	–4.909539	0.622808	0.367908
C	–4.399517	1.728189	–0.362277
C	–3.983100	1.510533	–1.717987
C	–3.051654	2.414481	–2.289650
C	–2.001257	1.897658	–3.084395
C	–0.844623	2.720718	–3.307768
C	0.442954	2.101464	–3.279977
C	1.600100	2.892500	–3.149251
C	2.692692	2.376645	–2.322174
C	3.658706	3.277420	–1.754220
C	4.028992	3.145520	–0.446433
H	–0.435762	–6.674820	0.163440
H	–1.065966	–6.362569	–2.155145
H	–2.679844	–5.591069	–3.349859
H	–4.858312	–4.559135	–3.362069
H	–6.479196	–3.769697	–2.156222
H	–7.178497	–3.405953	0.126567
H	–6.567064	–3.668728	2.201563
H	–4.781321	–4.507767	3.597808
H	–2.817453	–5.448576	3.630592
H	–1.032023	–6.338048	2.256684
H	2.228273	5.076849	3.492132
H	4.025027	4.212267	2.114245
H	4.628707	3.922381	0.016194
H	3.984874	4.149658	–2.310013
H	2.349021	4.906947	–3.496209
H	0.179033	5.957295	–3.509572
H	–1.439021	6.753915	–2.301245
H	–2.137395	7.120478	–0.018593
H	–1.518395	6.854084	2.056232
H	0.265876	6.017613	3.454493
C	3.605468	–2.046859	–0.639965
O	4.132835	–2.816694	0.137907
O	4.160450	–1.577153	–1.734120
H	5.161722	–1.839948	–1.764128
C	7.018813	–1.559855	–0.220917
C	6.243346	–0.281590	0.080860

(CC) 2018 SCS.

C	8.530559	–1.420596	0.126434
O	6.202481	0.549564	–0.965625
N	6.746804	–1.962829	–1.604024
S	8.598403	–1.027341	1.938269
O	5.735388	–0.042944	1.150195
C	9.214509	–0.310613	–0.673267
C	9.223382	–2.762190	–0.121634
H	6.583772	–2.321808	0.430947
H	5.674402	1.331792	–0.721585
H	7.095071	–2.900903	–1.781643
H	7.185963	–1.329187	–2.268932
H	9.921292	–1.223473	2.049430
H	10.270906	–0.255214	–0.397904
H	8.758657	0.664051	–0.489127
H	9.168313	–0.522183	–1.747435
H	10.262987	–2.718102	0.212740
H	9.237251	–2.995308	–1.191107
H	8.720842	–3.572514	0.413058

E = – 4429.107062

PCA

C	6.746884	1.426292	–0.578942
C	6.124139	0.340871	0.286150
C	8.183569	1.792298	–0.093512
O	6.040021	–0.839605	–0.331606
N	5.786635	2.520268	–0.593906
S	9.195449	0.251586	0.037206
O	5.713175	0.532133	1.408169
C	8.191823	2.412925	1.304623
C	8.826564	2.750221	–1.096530
H	6.836411	1.032179	–1.597096
H	5.633871	–1.470475	0.285778
H	6.130798	3.296574	–1.149696
H	5.634800	2.854434	0.353958
H	9.075508	–0.133075	–1.244678
H	9.216276	2.660467	1.594869
H	7.761136	1.742656	2.050520
H	7.614813	3.342177	1.297011
H	9.855392	2.969041	–0.802394
H	8.278074	3.697613	–1.124837
H	8.835302	2.324798	–2.104414

E = –800.204903

(CC) 2018 SCS.