

Photostability and Solvation: Photodynamics of Microsolvated Zwitterionic Glycine

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FC (1A)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.891442011	-0.603895706
3 N	7.00	0.000000000	0.000000000	2.826680480
4 O	8.00	1.288168888	3.602359603	-2.454481827
5 O	8.00	-1.264496134	4.127755736	1.035625327
6 O	8.00	4.896191264	1.960022121	1.621500660
7 H	1.00	1.650454679	-0.979635236	-0.720941507
8 H	1.00	-1.737142892	-0.882640684	-0.659980242
9 H	1.00	-0.757997581	-1.546923864	3.676684952
10 H	1.00	-1.029781701	1.712760973	3.105168521
11 H	1.00	1.823957406	0.315281641	3.409696676
12 H	1.00	6.230874937	2.997697531	2.301283841
13 H	1.00	4.338773395	2.808259344	0.081328453

CN (1A)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.712909173	-0.130747757
3 N	7.00	0.000000000	0.000000000	4.724314971
4 O	8.00	2.339666294	3.738687082	-0.340633219
5 O	8.00	-1.847216799	4.118789970	-0.002312439
6 O	8.00	4.955930075	3.366294152	5.769559097
7 H	1.00	1.741195206	-1.019829233	-0.054408577
8 H	1.00	-1.743898808	-0.985219504	0.235479144
9 H	1.00	-0.368444242	-1.620202652	5.641296370
10 H	1.00	-1.398097493	1.207919777	5.159787654
11 H	1.00	1.596173818	0.720653652	5.462593647
12 H	1.00	5.967186737	4.256090366	6.950434216
13 H	1.00	5.211215138	4.156311185	4.179236558

NPI (1A)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.768873242	-0.742588653
3 N	7.00	0.000000000	0.000000000	2.853952509
4 O	8.00	2.376292112	3.780163493	-0.749311091
5 O	8.00	-1.462325365	4.151595979	0.775822328
6 O	8.00	4.908925193	2.078699584	3.719094693
7 H	1.00	1.610842997	-1.063348089	-0.666313823
8 H	1.00	-1.736865615	-0.900219168	-0.581159809
9 H	1.00	-0.679188088	-1.587843114	3.643432506
10 H	1.00	-1.112961578	1.529054048	3.268451410

11 H	1.00	1.748550839	0.379036951	3.553281877
12 H	1.00	5.812736926	3.075212977	4.901616133
13 H	1.00	4.494442729	3.141022572	2.307585539

NH (1A)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.630880647	-1.175332663
3 N	7.00	0.000000000	0.000000000	2.712672819
4 O	8.00	0.043834530	2.601652943	-3.664313047
5 O	8.00	-0.114854026	4.618273020	-0.009852641
6 O	8.00	5.932194683	1.612955590	-1.325486100
7 H	1.00	1.672218435	-0.959997585	-0.675267708
8 H	1.00	-1.628755553	-1.035759727	-0.686275443
9 H	1.00	-0.277166445	-3.042873550	4.207446278
10 H	1.00	-1.416601281	1.029536894	3.433618766
11 H	1.00	1.616134644	0.718964211	3.388327814
12 H	1.00	7.410268826	2.026064407	-0.401833815
13 H	1.00	6.336364549	1.856105737	-3.054667143

REGER (1A)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.635965293	-1.057797091
3 N	7.00	0.000000000	0.000000000	2.775571330
4 O	8.00	2.112336985	4.043920703	-1.036133701
5 O	8.00	-2.146752268	4.050720601	-0.320164092
6 O	8.00	3.469882101	4.100032239	4.302494836
7 H	1.00	1.706693328	-0.918427494	-0.649459574
8 H	1.00	-1.602229809	-1.028381974	-0.773336086
9 H	1.00	0.341586085	-1.746351191	3.426858796
10 H	1.00	-1.704258628	0.504945549	3.433535585
11 H	1.00	2.407678250	2.633721658	4.315971442
12 H	1.00	2.875466205	5.212564394	5.573354273
13 H	1.00	2.671437255	4.432684224	0.683293251

S2MIN (1A)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.679410337	-0.975389511
3 N	7.00	0.000000000	0.000000000	2.770827606
4 O	8.00	-0.039865995	2.815529752	-3.467879821
5 O	8.00	0.018844037	4.563876036	0.340497433
6 O	8.00	5.249409342	2.022720889	1.259247664
7 H	1.00	1.666816055	-0.978161792	-0.641464472
8 H	1.00	-1.642037146	-1.018369127	-0.653060336
9 H	1.00	0.132844841	-1.826303705	3.423622138
10 H	1.00	-1.632275249	0.707586308	3.511391419
11 H	1.00	1.481849328	0.994818973	3.475749682
12 H	1.00	6.693068213	0.979004952	1.475756282
13 H	1.00	5.762083085	3.688535127	1.690777638

FC (2A)

1 C	6.00	3.250609751	1.803306807	-0.629559247
2 C	6.00	3.815250121	2.226740697	-3.488313827
3 N	7.00	2.114982572	-0.794528858	-0.364996701
4 O	8.00	5.976746074	1.513140442	-4.220660422
5 O	8.00	2.011368757	3.145495816	-4.761442218
6 O	8.00	6.488763308	-3.058321547	-2.049876610
7 O	8.00	-2.055071570	0.540316680	-3.178326763
8 H	1.00	4.979960901	1.851959898	0.493416813
9 H	1.00	1.873029032	3.167484708	0.074529664

10 H	1.00	1.695587056	-1.208180930	1.478784614
11 H	1.00	0.441189798	-0.862490138	-1.413598092
12 H	1.00	3.423272692	-2.123363322	-1.018755367
13 H	1.00	7.053422827	-4.430551341	-3.131277000
14 H	1.00	6.786302727	-1.452247664	-3.000448637
15 H	1.00	-0.901456810	1.775575600	-4.024763716
16 H	1.00	-3.164063408	-0.131456525	-4.478380251

CN (2A)

1 C	6.00	-2.707467106	-1.631820912	-0.966290016
2 C	6.00	-0.154586740	-2.243853503	-0.290700774
3 N	7.00	-2.041744731	2.902378581	0.181316464
4 O	8.00	1.704270957	-2.123937120	-1.602813989
5 O	8.00	0.167910761	-3.049077582	2.158897449
6 O	8.00	1.202176661	2.296623494	-4.999117517
7 O	8.00	1.194766435	2.321816897	5.300964665
8 H	1.00	-4.191330495	-1.685072933	0.399173891
9 H	1.00	-3.069399709	-1.027039294	-2.857918295
10 H	1.00	-3.685721021	3.850386645	0.173382944
11 H	1.00	-1.087152454	3.434017339	-1.373587543
12 H	1.00	-1.060447910	3.512776459	1.690108030
13 H	1.00	2.494564688	2.546041607	6.512160991
14 H	1.00	1.201425962	0.585698830	4.848643449
15 H	1.00	1.741969757	0.750085681	-4.252122690
16 H	1.00	2.368870837	2.687584657	-6.298941427

NPI (2A)

1 C	6.00	3.228140728	2.174913816	-0.432613704
2 C	6.00	3.874970842	2.758875448	-3.155790509
3 N	7.00	2.237420509	-0.511439013	-0.247363148
4 O	8.00	6.487520952	1.954642423	-3.651010836
5 O	8.00	2.346521515	2.062734447	-4.861768386
6 O	8.00	6.300156982	-3.346916092	-2.524009304
7 O	8.00	-2.146217647	0.347369167	-3.292556839
8 H	1.00	4.826087865	2.331263792	0.830680213
9 H	1.00	1.710162543	3.374029483	0.217177893
10 H	1.00	1.830410513	-1.006386595	1.543332317
11 H	1.00	0.626501367	-0.653161584	-1.293107747
12 H	1.00	3.514838995	-1.762978778	-0.956098247
13 H	1.00	6.214785757	-4.632007602	-3.769532541
14 H	1.00	6.821187488	-1.831874560	-3.364139092
15 H	1.00	-0.832440058	1.182419126	-4.266541531
16 H	1.00	-3.250159116	-0.478603078	-4.490324923

NH (2A)

1 C	6.00	-2.222764702	0.523501134	-0.163606334
2 C	6.00	-0.529041678	-1.708420178	-0.875302615
3 N	7.00	-0.915431098	2.652531534	0.874177548
4 O	8.00	-0.402903527	-2.707096918	-2.884090903
5 O	8.00	0.904664063	-2.487131679	1.095233216
6 O	8.00	1.624612116	2.282100000	-4.663319190
7 O	8.00	0.944207335	0.503438235	6.116660941
8 H	1.00	-3.613245191	-0.149189653	1.182502236
9 H	1.00	-3.191954913	1.059402990	-1.879105729
10 H	1.00	-3.115072659	5.196302685	1.385112231
11 H	1.00	0.373711456	3.343780054	-0.327405516
12 H	1.00	-0.141513964	2.313624693	2.567354516
13 H	1.00	0.975655210	1.061139743	7.819254546
14 H	1.00	1.925750062	-0.995852280	6.043076448

15 H	1.00	1.253340882	0.583168212	-5.119189072
16 H	1.00	2.305636065	3.081049692	-6.113692295

REGER (2A)

1 C	6.00	-0.478683618	-1.443749975	-3.273710053
2 C	6.00	1.098299636	0.750368295	-2.394221487
3 N	7.00	-1.963778586	-2.573698421	-1.230055886
4 O	8.00	0.030077446	2.904526079	-1.615993737
5 O	8.00	3.078744245	0.016270938	-0.708398766
6 O	8.00	-2.921666196	1.517560197	2.595321459
7 O	8.00	1.460201438	-1.091674691	4.806027309
8 H	1.00	0.750111708	-2.804075313	-4.205110073
9 H	1.00	-1.770874148	-0.712609396	-4.679969093
10 H	1.00	-3.276503219	-3.739778711	-1.939878258
11 H	1.00	-3.317255519	0.033667698	1.648792577
12 H	1.00	-0.867450672	-3.612283717	-0.084611461
13 H	1.00	2.571235730	-1.120887739	6.210780407
14 H	1.00	2.458385508	-0.786639771	3.341213749
15 H	1.00	-1.000029066	2.685497974	-0.126896347
16 H	1.00	-1.790921420	0.961649997	3.881844815

S2MIN (2A)

1 C	6.00	3.388261992	2.091597082	-0.489782413
2 C	6.00	3.981212238	2.899568269	-3.203696820
3 N	7.00	2.230370811	-0.537878396	-0.432250556
4 O	8.00	5.546543461	1.250854664	-4.217400945
5 O	8.00	1.786150466	3.594999886	-4.300880781
6 O	8.00	6.509468834	-3.463610149	-2.166944331
7 O	8.00	-2.218548043	0.226351266	-3.461202657
8 H	1.00	5.092016191	1.986460873	0.625171699
9 H	1.00	2.045788745	3.336691389	0.404266926
10 H	1.00	1.775432432	-1.065353813	1.338489082
11 H	1.00	0.629629223	-0.600357443	-1.496910896
12 H	1.00	3.476655022	-1.824206165	-1.123947961
13 H	1.00	7.189398745	-4.913746490	-2.966885222
14 H	1.00	6.803247658	-2.037409038	-3.246721459
15 H	1.00	-1.267683109	1.574978085	-4.219985278
16 H	1.00	-3.178051292	-0.556059828	-4.754985867

FC (2B)

1 C	6.00	2.184416062	2.122212243	-0.594208499
2 C	6.00	2.049421080	-0.759368884	-0.037007810
3 O	8.00	2.854519105	-2.208201480	-1.701165137
4 O	8.00	1.041885925	-1.252187148	2.124176907
5 O	8.00	-4.092457152	1.520905720	-0.995472563
6 O	8.00	-3.187828979	-3.465625478	0.096682476
7 N	7.00	0.311878467	3.316116555	1.159175907
8 H	1.00	1.683273132	2.525350184	-2.550286740
9 H	1.00	4.068585581	2.855118767	-0.175130028
10 H	1.00	0.700910297	5.140024678	1.661861888
11 H	1.00	-1.502804916	3.150259608	0.403733271
12 H	1.00	0.337046682	2.054658253	2.693058596
13 H	1.00	-5.889316976	1.876418101	-1.118622103
14 H	1.00	-2.588957981	-4.530227861	-1.278630727
15 H	1.00	-3.932249495	-0.340769417	-0.721822734
16 H	1.00	-1.655049854	-3.140891097	1.125017856

CN (2B)

1 C	6.00	0.000000000	0.000000000	0.000000000
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2	C	6.00	0.000000000	2.706244738	-0.107889193
3	N	7.00	0.000000000	0.000000000	4.724314971
4	O	8.00	1.871605363	4.097686151	-0.038954337
5	O	8.00	-2.284798464	3.760214693	-0.323822090
6	O	8.00	1.699155183	8.514286077	3.393554266
7	O	8.00	-0.604840170	5.413265293	7.278503233
8	H	1.00	-1.733757800	-1.031922099	0.034281835
9	H	1.00	1.769462360	-0.961964723	0.104731549
10	H	1.00	-0.938280786	-1.462591750	5.487990208
11	H	1.00	-0.519573987	1.559635767	5.684580836
12	H	1.00	1.836626719	-0.265016171	5.124491829
13	H	1.00	-0.313144612	6.096064727	8.906799968
14	H	1.00	0.938690363	9.947747394	2.635314496
15	H	1.00	0.143705849	6.553475917	6.093301584
16	H	1.00	1.966492978	7.312910803	2.076464393

NPI (2B)

1	C	6.00	0.000000000	0.000000000	0.000000000
2	C	6.00	0.000000000	2.798133123	-0.678232450
3	N	7.00	0.000000000	0.000000000	2.818342897
4	O	8.00	1.525394019	4.141945995	0.821592418
5	O	8.00	0.461277835	3.170593738	-3.180474419
6	O	8.00	-1.633778856	7.232565864	3.560841910
7	O	8.00	-3.967231853	2.768494740	5.140586344
8	H	1.00	-1.622867078	-1.037493575	-0.676606912
9	H	1.00	1.725567996	-0.927323833	-0.609269392
10	H	1.00	0.473750921	-1.670485904	3.586729790
11	H	1.00	-1.674247872	0.597623080	3.558028302
12	H	1.00	1.279105644	1.365870346	3.281866959
13	H	1.00	-5.199329682	2.923308631	6.430210439
14	H	1.00	-2.306004246	8.579721879	2.591572648
15	H	1.00	-3.440873271	4.452165571	4.679309567
16	H	1.00	-0.392121127	6.400513229	2.500484578

NH (2B)

1	C	6.00	0.000000000	0.000000000	0.000000000
2	C	6.00	0.000000000	2.572409455	-1.310701460
3	N	7.00	0.000000000	0.000000000	2.704882273
4	O	8.00	0.078271627	4.662312937	-0.273718211
5	O	8.00	0.032899651	2.474824753	-3.798787443
6	O	8.00	-4.225907142	7.733048554	1.975498953
7	O	8.00	-5.544462002	2.444385524	2.331357427
8	H	1.00	-1.617939275	-1.034052913	-0.694584603
9	H	1.00	1.674348351	-0.979590928	-0.678800500
10	H	1.00	1.215373702	-2.838779488	4.131222399
11	H	1.00	-1.663569278	0.655174926	3.335042331
12	H	1.00	1.365774710	1.102527348	3.414759204
13	H	1.00	-7.120858209	2.073503461	3.096262561
14	H	1.00	-4.855710708	9.073037586	0.967850623
15	H	1.00	-5.404002993	4.244321666	2.271343934
16	H	1.00	-2.550812096	7.397639866	1.418734935

REGER (2B)

1	C	6.00	0.000000000	0.000000000	0.000000000
2	C	6.00	0.000000000	2.725013163	-0.859864302
3	N	7.00	0.000000000	0.000000000	2.745481553
4	O	8.00	1.580212592	4.338921842	0.558136655
5	O	8.00	0.444463887	3.118457481	-3.335597201
6	O	8.00	-2.509526508	7.705528741	2.608459362

7 O	8.00	-4.862368332	3.017429676	4.272480114
8 H	1.00	-1.595389287	-0.977987842	-0.844202989
9 H	1.00	1.720593927	-0.906610686	-0.663863791
10 H	1.00	0.463300954	-1.696723551	3.437718459
11 H	1.00	-1.693978858	0.498365374	3.445126312
12 H	1.00	1.835846294	3.440514694	2.115213370
13 H	1.00	-5.903748100	3.233487943	5.712405334
14 H	1.00	-3.210453936	8.898594961	1.470531543
15 H	1.00	-4.306203840	4.666086074	3.783616871
16 H	1.00	-1.053015211	7.013494006	1.802474290

S2MIN (2B)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.634321434	-1.079486905
3 N	7.00	0.000000000	0.000000000	2.768357337
4 O	8.00	-0.048103406	4.589349688	0.176115193
5 O	8.00	0.038353310	2.721048565	-3.569409902
6 O	8.00	-4.748030111	7.399700424	1.757377352
7 O	8.00	-4.962424555	2.232708663	3.383353239
8 H	1.00	-1.665536556	-0.996933430	-0.635190397
9 H	1.00	1.635664332	-1.030121471	-0.658763333
10 H	1.00	0.280422472	-1.821194615	3.398606296
11 H	1.00	-1.666019356	0.657731861	3.474069314
12 H	1.00	1.450801857	1.028702550	3.503642617
13 H	1.00	-6.396727600	1.692873498	4.312488966
14 H	1.00	-5.627847934	8.706444491	0.901507881
15 H	1.00	-5.227499626	3.965467354	2.940485317
16 H	1.00	-3.009594721	7.565044433	1.331915732

FC (2C)

1 C	6.00	2.846423694	-2.045740311	3.048153550
2 C	6.00	3.538114882	0.784007496	2.658400796
3 H	1.00	3.946169689	-2.823738705	4.611310888
4 H	1.00	0.838195767	-2.218441935	3.490226580
5 H	1.00	2.364335641	-2.856681278	-0.797101105
6 H	1.00	5.293958036	-3.426368033	0.258981920
7 H	1.00	2.936615743	-5.446266379	0.963561209
8 H	1.00	9.939875325	-1.683005329	0.105190633
9 H	1.00	7.338964624	-0.262639239	-0.315073731
10 H	1.00	-0.272216918	0.301969293	-3.575081022
11 H	1.00	2.314052489	0.714011044	-2.125818735
12 N	7.00	3.386414086	-3.579251288	0.722984181
13 O	8.00	4.436618060	1.345898300	0.465221871
14 O	8.00	3.131317310	2.142492770	4.524911066
15 O	8.00	8.232398725	-1.899512067	-0.534098377
16 O	8.00	1.267564377	-0.545649516	-3.044370092

CN (2C)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.705071461	0.116078541
3 N	7.00	0.000000000	0.000000000	4.724314971
4 O	8.00	2.240588315	3.808289943	-0.174690523
5 O	8.00	-1.854593726	4.086908473	0.476400286
6 O	8.00	-5.828296097	0.591712102	2.492474135
7 O	8.00	-0.891842117	6.031214965	5.860072880
8 H	1.00	1.740013884	-1.018721124	-0.095200782
9 H	1.00	-1.760221827	-0.969896057	0.171026085
10 H	1.00	-1.865690742	-0.352141947	4.800475311
11 H	1.00	0.287339843	1.546364345	5.793732850

12 H	1.00	0.871893763	-1.442446141	5.597610202
13 H	1.00	-0.784457940	7.741473729	6.377763744
14 H	1.00	-1.338994844	6.039195412	4.120261071
15 H	1.00	-7.577567733	0.953962948	2.604152594
16 H	1.00	-5.025353281	2.048428308	1.805829808

NPI (2C)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.751982278	-0.829340793
3 N	7.00	0.000000000	0.000000000	2.830905598
4 O	8.00	-0.250042881	2.937682215	-3.385279619
5 O	8.00	-1.593926021	4.252937151	0.421776948
6 O	8.00	-5.093647815	1.597765432	3.088096787
7 O	8.00	1.466373247	4.880167905	4.603402060
8 H	1.00	1.653654321	-1.013839602	-0.643033185
9 H	1.00	-1.687011756	-1.000370169	-0.597809025
10 H	1.00	-1.771393128	0.433760229	3.453480168
11 H	1.00	1.153998569	1.372588815	3.530059074
12 H	1.00	0.502638860	-1.682699044	3.556375726
13 H	1.00	2.760143684	6.115998360	4.664216404
14 H	1.00	0.419206080	5.257846960	3.154732577
15 H	1.00	-6.282779843	2.424931422	4.140040870
16 H	1.00	-4.354307828	2.852357553	1.981064822

NH (2C)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.548206754	-1.294935799
3 N	7.00	0.000000000	0.000000000	2.711294187
4 O	8.00	-0.000405291	2.544631859	-3.771350397
5 O	8.00	0.000464120	4.621010182	-0.165062664
6 O	8.00	-4.924577966	3.521092408	2.848620155
7 O	8.00	4.916736076	3.531322348	2.862179682
8 H	1.00	1.636639056	-1.026651482	-0.684811987
9 H	1.00	-1.636783540	-1.026421517	-0.684745613
10 H	1.00	-1.538831614	0.858708462	3.401298399
11 H	1.00	1.538521664	0.858997227	3.401661381
12 H	1.00	0.000271906	-3.333412638	3.388500567
13 H	1.00	6.588043602	3.871554236	3.410108385
14 H	1.00	4.171126558	5.109640627	2.449483068
15 H	1.00	-6.598714556	3.851599628	3.393892720
16 H	1.00	-4.186143373	5.104247569	2.441599426

REGER (2C)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.656201744	-1.017192526
3 N	7.00	0.000000000	0.000000000	2.754251834
4 O	8.00	-0.047478099	2.819855944	-3.545466967
5 O	8.00	1.809341675	4.423714271	-0.143286363
6 O	8.00	-1.271652184	5.720116509	4.447190088
7 O	8.00	5.117319083	1.826894933	3.087085281
8 H	1.00	1.677406960	-0.988838950	-0.662385919
9 H	1.00	-1.628748189	-0.957340092	-0.810566422
10 H	1.00	-1.298898345	1.192420083	3.456818966
11 H	1.00	3.576682716	1.051762392	3.651322484
12 H	1.00	-0.390939325	-1.731068731	3.412666394
13 H	1.00	5.793736359	2.750468761	4.464941478
14 H	1.00	3.193256782	3.570130625	0.679487560
15 H	1.00	-2.144212486	7.269620576	4.653083066
16 H	1.00	-0.292030496	5.865442018	2.944272365

S2MIN (2C)

1	C	6.00	0.000000000	0.000000000	0.000000000
2	C	6.00	0.000000000	2.613076069	-1.132169165
3	N	7.00	0.000000000	0.000000000	2.769309079
4	O	8.00	-0.058233787	2.686672644	-3.627153217
5	O	8.00	-0.002505783	4.609890202	0.112155482
6	O	8.00	-4.067593032	3.644197191	4.239711431
7	O	8.00	3.875119437	3.782126341	4.345893906
8	H	1.00	1.612116819	-1.076219498	-0.647086409
9	H	1.00	-1.664569578	-1.003000822	-0.635221776
10	H	1.00	-1.559399218	0.855511337	3.492474681
11	H	1.00	1.556309982	0.843539156	3.510107959
12	H	1.00	-0.015033442	-1.860093131	3.348756557
13	H	1.00	5.648546360	3.883890450	4.577579442
14	H	1.00	3.366843633	5.246258399	3.449578650
15	H	1.00	-5.850819025	3.587420870	4.400241125
16	H	1.00	-3.676791933	5.101358016	3.275103863

FC (2D)

1	C	6.00	2.046332425	-1.746231756	2.849973539
2	C	6.00	3.435533713	0.823568127	2.470509781
3	N	7.00	3.156475514	-3.392637999	0.834507012
4	O	8.00	5.792311031	0.539197260	2.165676902
5	O	8.00	2.055490293	2.764120894	2.357052370
6	O	8.00	0.548856353	0.201863196	-2.177011575
7	O	8.00	2.182935347	-8.789057829	1.594509953
8	H	1.00	2.495536024	-2.572997483	4.687651098
9	H	1.00	0.008798660	-1.616462446	2.578970529
10	H	1.00	2.452711585	-2.735220001	-0.869065204
11	H	1.00	5.067400584	-2.946543380	0.892858204
12	H	1.00	2.831038254	-5.299254505	1.047746163
13	H	1.00	0.725018383	1.072430045	-3.784041006
14	H	1.00	0.767656636	1.513190181	-0.859696987
15	H	1.00	3.343636386	-10.048723447	2.266612137
16	H	1.00	0.539207607	-9.612398432	1.514575495

CN (2D)

1	C	6.00	0.000000000	0.000000000	0.000000000
2	C	6.00	0.000000000	2.714918872	-0.129783680
3	N	7.00	0.000000000	0.000000000	4.724314971
4	O	8.00	-1.812880453	4.098077537	-0.159698924
5	O	8.00	2.339680678	3.797975974	-0.258043766
6	O	8.00	-7.082648058	3.055541763	0.974798652
7	O	8.00	-5.812303282	-1.307590512	3.919352853
8	H	1.00	1.730514390	-1.033052447	0.104143992
9	H	1.00	-1.777462903	-0.956898282	0.059679799
10	H	1.00	0.273476341	1.216937277	6.157125924
11	H	1.00	1.005046528	-1.553304348	5.149235356
12	H	1.00	-1.833353971	-0.502200781	4.773815419
13	H	1.00	-7.885266242	4.560325460	1.521716400
14	H	1.00	-5.424029299	3.521150443	0.433243805
15	H	1.00	-7.141737417	-2.495745820	4.078330468
16	H	1.00	-6.486362204	0.113162262	3.025101516

NPI (2D)

1	C	6.00	0.000000000	0.000000000	0.000000000
2	C	6.00	0.000000000	2.783565342	-0.754822322
3	N	7.00	0.000000000	0.000000000	2.842371479

4 O	8.00	-2.611033340	3.709115922	-0.974174270
5 O	8.00	1.246808534	4.220181715	0.693833306
6 O	8.00	-5.073276194	1.886159811	3.520744086
7 O	8.00	2.673559630	-4.517074732	4.991635950
8 H	1.00	1.737879211	-0.897425600	-0.584415488
9 H	1.00	-1.601888047	-1.071519970	-0.673440536
10 H	1.00	-1.765086881	0.291451249	3.529601591
11 H	1.00	1.026887779	1.578375982	3.274745415
12 H	1.00	0.769264459	-1.558540700	3.627333533
13 H	1.00	-5.932198929	2.943367412	4.683441899
14 H	1.00	-4.670408062	2.898817443	2.071427281
15 H	1.00	4.444039902	-4.527170555	5.283340913
16 H	1.00	2.073533343	-6.148835322	5.433132066

NH (2D)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.667952177	-1.049636422
3 N	7.00	0.000000000	0.000000000	2.738819200
4 O	8.00	-1.661628505	3.418946091	-2.517716512
5 O	8.00	1.810176104	4.189090162	-0.436515169
6 O	8.00	-5.602341817	2.492549468	1.736687127
7 O	8.00	2.293798479	-5.426175081	3.344545848
8 H	1.00	1.713007231	-0.923509394	-0.643509459
9 H	1.00	-1.591168532	-0.994078843	-0.828801250
10 H	1.00	-1.681524373	0.583266617	3.391659921
11 H	1.00	2.615737406	1.149201469	4.584761284
12 H	1.00	0.290407058	-1.766773881	3.353405182
13 H	1.00	-6.788410354	3.491928547	2.631732768
14 H	1.00	-5.620230724	3.064294565	0.036346194
15 H	1.00	3.997660427	-5.058974028	3.768859163
16 H	1.00	2.054115891	-7.162704080	3.717823859

REGER (2D)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.684416675	-0.949263382
3 N	7.00	0.000000000	0.000000000	2.751163131
4 O	8.00	-2.461662762	3.735065511	-1.199609681
5 O	8.00	1.556788253	4.332444883	0.206669490
6 O	8.00	-5.632413554	2.115586091	3.241094540
7 O	8.00	3.384338780	-4.789939589	4.216408813
8 H	1.00	1.724829117	-0.892948772	-0.645200791
9 H	1.00	-1.577396809	-1.015757055	-0.838104895
10 H	1.00	-1.748259129	0.216704548	3.449061304
11 H	1.00	1.762716974	3.767950821	1.951755523
12 H	1.00	0.726705951	-1.610991606	3.427302830
13 H	1.00	-7.239541226	2.694165193	3.776636280
14 H	1.00	-5.102950831	3.183937134	1.896102618
15 H	1.00	4.888566661	-4.221976586	5.009315910
16 H	1.00	3.333942463	-6.568061869	4.433487577

S2MIN (2D)

1 C	6.00	0.000000000	0.000000000	0.000000000
2 C	6.00	0.000000000	2.754064984	-0.882841906
3 N	7.00	0.000000000	0.000000000	2.827658339
4 O	8.00	-1.890950472	4.024718413	-0.684980571
5 O	8.00	2.548701716	3.768782262	1.210803661
6 O	8.00	-4.777450147	2.532675683	3.484360758
7 O	8.00	1.151328779	-5.134270271	4.859001740
8 H	1.00	1.675240565	-0.983754095	-0.610415259

Supplementary Material (ESI) for *PCCP*

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9 H	1.00	-1.680622220	-0.967119434	-0.644957773
10 H	1.00	-1.657919175	0.703291639	3.498442749
11 H	1.00	1.408009060	1.205133028	3.367498612
12 H	1.00	0.310725237	-1.735913429	3.559936613
13 H	1.00	-5.385432811	3.752072132	4.646774128
14 H	1.00	-4.256435413	3.432408144	1.994626807
15 H	1.00	2.808548202	-5.756789556	5.152056457
16 H	1.00	0.019691644	-6.433355149	5.359350114