Ene-diamine vs. Imine-amine Isomeric Preferences

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Supporting Information

Supporting Information Available: Compound characterization data, including NMR spectra, X-ray crystallographic data (**13-E**, **13-Me₂-E**, and **17a**), and DFT zero point energies and Cartesian coordinates for all relevant computationally studied species.

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¹H NMR spectra

N-benzylideneaniline (**11**), CDCl₃, RT, [538-51-2]

N-benzylidenetoluidine (**11-Me**), CDCl₃, RT, [2272-45-9]

N,N'-bis(salicylidene)-*o*-phenylenediamine (**16**, salophen), CDCl₃, RT, [3946-91-6]

1,2,*N,N'*-tetraphenylethylene-1,2-diamine (**13**), CDCl₃, -60°C, [24099-48-7]

1,2,*N,N'*-tetraphenylethylene-1,2-diamine (**13**), CDCl₃, 60°C, [24099-48-7]

1,2-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (**13-Me**₂), CDCl₃, -60°C, [24099-52-3]

1,2-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (**13-Me₂**), CDCl₃, 60°C, [24099-52-3]

(+/-)-2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline (**17**), acetone-*d*₆, RT, [671210-48-3]

Average bond dissociation energy calculations¹

hydroxy-ketone vs. ene-diol

bonds broken	energy (kcal/mol)
C=O	172
C-C	81
C-H	100

bonds made	energy (kcal/mol)
C-O	84
C=C	148
O-H	110

$$\Delta H = 172 + 81 + 100 - (84 + 148 + 110) = +11 \text{ kcal/mol}$$

imine-amine vs. ene-diamine

bonds broken	energy (kcal/mol)
C=N	148
C-C	81
C-H	100

bonds made	energy (kcal/mol)
C-N	69
C=C	148
N-H	93

$$\Delta H = 148 + 81 + 100 - (69 + 148 + 93) = +19 \text{ kcal/mol}$$

Computational methods

All calculations were performed using the Gaussian 03 suite of programs.² Optimized structure calculations and frequency calculations were performed using Density Function Theory (DFT) employing the Becke's 3-parameter hybrid functional (B3)³ with the correlation functional of Lee, Yang and Parr (LYP)^{4,5}. The Pople style basis sets, 6-31+G(d') and 6-311++G(d,p) were used. Restricted calculations were performed, as all relevant species were closed shell molecules.

DFT structures and coordinates: Figure 5

benzoin (2)
B3LYP/6-31+G(d')

1	O	0.121	1.724	1.971
2	O	-1.588	-0.145	2.550
3	C	1.309	0.656	0.219
4	C	2.223	1.723	0.128
5	C	3.281	1.672	-0.778
6	C	3.442	0.551	-1.604
7	C	2.540	-0.515	-1.519
8	C	1.479	-0.464	-0.613
9	C	-1.795	-0.373	0.143
10	C	-2.405	0.803	-0.322
11	C	-3.290	0.763	-1.400
12	C	-3.578	-0.454	-2.031
13	C	-2.980	-1.631	-1.570
14	C	-2.094	-1.587	-0.488
15	C	0.210	0.759	1.221
16	C	-0.863	-0.346	1.354
17	H	2.087	2.583	0.777
18	H	3.981	2.502	-0.842
19	H	4.268	0.510	-2.311
20	H	2.662	-1.386	-2.160
21	H	0.783	-1.296	-0.567
22	H	-2.194	1.753	0.167
23	H	-3.755	1.682	-1.752
24	H	-4.268	-0.484	-2.873
25	H	-3.206	-2.583	-2.046
26	H	-1.641	-2.509	-0.124
27	H	-1.354	0.745	2.874
28	H	-0.358	-1.319	1.430

Z-stilbenediol (3-Z)
B3LYP/6-31+G(d')

1	O	3.868	0.343	0.095
2	C	2.080	-0.974	-0.746
3	C	2.678	-2.165	-0.290

4	C	2.292	-3.400	-0.815
5	C	1.314	-3.469	-1.815
6	C	0.732	-2.288	-2.291
7	C	1.115	-1.052	-1.766
8	C	2.524	0.316	-0.182
9	H	3.445	-2.113	0.478
10	H	2.759	-4.312	-0.446
11	H	1.017	-4.431	-2.227
12	H	-0.013	-2.327	-3.083
13	H	0.674	-0.139	-2.161
14	H	4.072	1.215	0.470
15	O	2.535	2.556	0.406
16	C	0.319	1.619	-0.016
17	C	-0.206	2.816	-0.548
18	C	-1.585	3.043	-0.574
19	C	-2.467	2.082	-0.068
20	C	-1.956	0.895	0.472
21	C	-0.579	0.669	0.508
22	C	1.779	1.429	0.050
23	H	0.473	3.559	-0.964
24	H	-1.970	3.969	-0.998
25	H	-3.541	2.258	-0.089
26	H	-2.633	0.148	0.882
27	H	-0.190	-0.246	0.947
28	H	2.035	3.100	1.029

E-stilbenediol (**3-E**)
B3LYP/6-31+G(d')

1	O	0.549	0.100	1.958
2	C	-0.167	1.878	0.559
3	C	0.474	2.830	1.380
4	C	0.145	4.183	1.292
5	C	-0.835	4.619	0.393
6	C	-1.496	3.683	-0.409
7	C	-1.171	2.326	-0.325
8	C	0.197	0.452	0.667
9	H	1.228	2.493	2.085
10	H	0.656	4.902	1.932
11	H	-1.091	5.675	0.328
12	H	-2.280	4.005	-1.092
13	H	-1.734	1.605	-0.914
14	H	1.029	-0.742	1.949
15	O	0.145	-0.020	-1.692
16	C	0.580	-1.861	-0.259
17	C	1.364	-2.492	-1.247
18	C	1.668	-3.851	-1.157
19	C	1.190	-4.615	-0.085

20	C	0.391	-4.008	0.889
21	C	0.082	-2.648	0.800
22	C	0.271	-0.423	-0.375
23	H	1.729	-1.903	-2.084
24	H	2.280	-4.316	-1.928
25	H	1.428	-5.675	-0.019
26	H	-0.011	-4.598	1.710
27	H	-0.588	-2.205	1.535
28	H	0.215	0.945	-1.748

DFT structures and coordinates: Figure 6

E-ene-diamine (**13-E**)
B3LYP/6-31+G(d')

1	C	2.005	0.977	-2.672
2	C	1.146	0.190	-1.881
3	C	0.902	-1.140	-2.281
4	C	1.511	-1.667	-3.422
5	C	2.373	-0.877	-4.193
6	C	2.615	0.448	-3.812
7	C	0.492	0.772	-0.677
8	C	0.419	0.117	0.527
9	C	-0.309	0.662	1.707
10	C	0.277	0.611	2.986
11	C	-0.398	1.106	4.104
12	C	-1.678	1.656	3.970
13	C	-2.279	1.702	2.705
14	C	-1.603	1.209	1.587
15	N	1.233	-1.012	0.762
16	C	0.798	-2.263	1.232
17	C	1.757	-3.279	1.412
18	C	1.381	-4.539	1.875
19	C	0.042	-4.814	2.184
20	C	-0.911	-3.808	2.006
21	C	-0.549	-2.545	1.527
22	N	0.141	2.138	-0.754
23	C	-0.753	2.711	-1.675
24	C	-1.430	1.962	-2.655
25	C	-2.296	2.600	-3.550
26	C	-2.520	3.977	-3.480
27	C	-1.859	4.722	-2.494
28	C	-0.980	4.100	-1.606
29	H	2.060	-1.061	0.180
30	H	0.195	2.635	0.125
31	H	2.803	-3.071	1.188
32	H	2.141	-5.309	2.002
33	H	-0.249	-5.795	2.552

34	H	-1.958	-4.004	2.232
35	H	-1.309	-1.784	1.381
36	H	1.268	0.177	3.096
37	H	0.074	1.060	5.084
38	H	-2.208	2.036	4.842
39	H	-3.279	2.114	2.589
40	H	-2.085	1.231	0.612
41	H	-1.284	0.888	-2.717
42	H	-2.807	2.002	-4.303
43	H	-3.200	4.464	-4.177
44	H	-2.021	5.795	-2.419
45	H	-0.460	4.690	-0.853
46	H	0.219	-1.757	-1.700
47	H	1.303	-2.695	-3.715
48	H	2.843	-1.287	-5.084
49	H	3.278	1.074	-4.407
50	H	2.189	2.009	-2.384

Z-ene-diamine (**13-Z**)
B3LYP/6-31+G(d')

1	C	-2.400	1.471	1.381
2	C	-3.216	2.600	1.492
3	C	-3.175	3.599	0.512
4	C	-2.315	3.453	-0.583
5	C	-1.499	2.326	-0.693
6	C	2.459	-1.664	-0.118
7	C	3.210	-1.102	0.931
8	C	4.408	-1.700	1.333
9	C	4.875	-2.867	0.721
10	C	4.120	-3.436	-0.314
11	C	-0.660	0.114	0.194
12	C	2.931	-2.841	-0.735
13	C	1.517	1.323	-0.295
14	C	1.499	2.326	0.693
15	C	2.315	3.453	0.583
16	C	3.175	3.598	-0.512
17	C	3.216	2.600	-1.492
18	C	2.401	1.471	-1.381
19	C	0.660	0.114	-0.195
20	C	-2.459	-1.664	0.118
21	C	-2.931	-2.841	0.735
22	C	-4.120	-3.436	0.314
23	C	-4.875	-2.867	-0.721
24	C	-4.409	-1.700	-1.333
25	C	-3.210	-1.102	-0.931
26	C	-1.517	1.323	0.295
27	N	-1.250	-1.112	0.571

28	N	1.250	-1.112	-0.571
29	H	-2.441	0.694	2.141
30	H	-3.886	2.698	2.344
31	H	-3.814	4.476	0.596
32	H	-2.285	4.216	-1.359
33	H	-0.843	2.216	-1.553
34	H	2.860	-0.204	1.430
35	H	4.976	-1.246	2.144
36	H	5.806	-3.328	1.044
37	H	4.462	-4.346	-0.804
38	H	2.361	-3.281	-1.553
39	H	0.843	2.216	1.553
40	H	2.285	4.216	1.359
41	H	3.814	4.476	-0.596
42	H	3.886	2.698	-2.344
43	H	2.441	0.694	-2.141
44	H	-2.361	-3.281	1.552
45	H	-4.462	-4.346	0.804
46	H	-5.806	-3.328	-1.043
47	H	-4.976	-1.246	-2.143
48	H	-2.860	-0.204	-1.430
49	H	-0.625	-1.768	1.021
50	H	0.625	-1.768	-1.021

E-imine-amine (**14-E**)
B3LYP/6-31+G(d')

1	C	-0.559	0.684	-0.600
2	C	0.936	0.324	-0.630
3	N	-1.229	0.344	-1.637
4	C	-1.093	1.436	0.585
5	C	1.206	-1.008	0.096
6	N	1.741	1.433	-0.137
7	C	-2.630	0.469	-1.754
8	C	2.980	1.771	-0.680
9	C	-3.146	1.088	-2.906
10	C	-4.527	1.174	-3.103
11	C	-5.410	0.609	-2.176
12	C	-4.900	-0.040	-1.047
13	C	-3.520	-0.107	-0.830
14	C	0.620	-2.189	-0.391
15	C	0.852	-3.413	0.242
16	C	1.678	-3.475	1.370
17	C	2.272	-2.305	1.855
18	C	2.037	-1.079	1.221
19	C	-1.759	2.660	0.383
20	C	-2.242	3.394	1.469
21	C	-2.077	2.913	2.771
22	C	-1.417	1.698	2.984
23	C	-0.917	0.969	1.900

24	C	3.504	3.063	-0.458
25	C	4.752	3.423	-0.963
26	C	5.513	2.512	-1.707
27	C	5.000	1.230	-1.927
28	C	3.753	0.853	-1.420
29	H	1.152	0.165	-1.695
30	H	1.226	2.203	0.266
31	H	-2.451	1.498	-3.637
32	H	-4.911	1.670	-3.993
33	H	-6.486	0.663	-2.339
34	H	-5.576	-0.497	-0.327
35	H	-3.128	-0.618	0.046
36	H	-0.020	-2.145	-1.270
37	H	0.390	-4.318	-0.148
38	H	1.862	-4.428	1.863
39	H	2.925	-2.344	2.725
40	H	2.504	-0.171	1.592
41	H	-1.896	3.034	-0.629
42	H	-2.751	4.341	1.294
43	H	-2.460	3.481	3.617
44	H	-1.285	1.316	3.993
45	H	-0.402	0.029	2.075
46	H	2.919	3.785	0.113
47	H	5.129	4.428	-0.779
48	H	6.485	2.796	-2.103
49	H	5.578	0.503	-2.496
50	H	3.393	-0.158	-1.584

Z-imine-amine (**14-Z**)
B3LYP/6-31+G(d')

1	C	-2.645	0.244	0.644
2	C	-1.277	-0.472	0.592
3	N	-2.779	1.521	0.598
4	C	-3.897	-0.567	0.773
5	C	-1.029	-1.196	-0.742
6	N	-1.116	-1.314	1.776
7	C	-1.728	2.454	0.581
8	C	0.034	-1.311	2.568
9	C	-0.849	2.606	1.671
10	C	0.122	3.615	1.656
11	C	0.237	4.476	0.561
12	C	-0.644	4.332	-0.519
13	C	-1.629	3.343	-0.504
14	C	-1.305	-0.546	-1.955
15	C	-1.037	-1.172	-3.177

16	C	-0.487	-2.457	-3.203
17	C	-0.204	-3.109	-2.000
18	C	-0.474	-2.482	-0.776
19	C	-3.938	-1.949	0.505
20	C	-5.130	-2.669	0.645
21	C	-6.300	-2.023	1.054
22	C	-6.271	-0.650	1.324
23	C	-5.086	0.070	1.186
24	C	-0.047	-1.746	3.908
25	C	1.090	-1.791	4.710
26	C	2.338	-1.398	4.208
27	C	2.423	-0.966	2.882
28	C	1.292	-0.926	2.063
29	H	-0.529	0.324	0.655
30	H	-1.970	-1.545	2.267
31	H	-0.943	1.948	2.533
32	H	0.791	3.720	2.507
33	H	0.994	5.256	0.553
34	H	-0.573	5.004	-1.374
35	H	-2.334	3.248	-1.328
36	H	-1.733	0.454	-1.950
37	H	-1.263	-0.654	-4.108
38	H	-0.280	-2.945	-4.153
39	H	0.230	-4.108	-2.006
40	H	-0.256	-2.991	0.160
41	H	-3.045	-2.469	0.169
42	H	-5.139	-3.735	0.423
43	H	-7.225	-2.586	1.162
44	H	-7.178	-0.138	1.648
45	H	-5.057	1.137	1.393
46	H	-1.014	-2.046	4.315
47	H	1.000	-2.130	5.743
48	H	3.226	-1.431	4.839
49	H	3.384	-0.663	2.467
50	H	1.394	-0.615	1.025

imine-amine (**17a**)
B3LYP/6-31+G(d')

1	O	3.277	-0.668	0.568
2	H	4.089	-0.813	0.064
3	O	-3.264	-0.929	3.410
4	H	-2.731	-0.104	3.229
5	N	1.443	0.806	2.477
6	H	2.434	0.908	2.300
7	N	-1.281	0.554	2.650

8	C	0.852	-0.375	1.838
9	H	1.441	-1.224	2.195
10	C	-0.583	-0.508	2.356
11	C	0.695	1.973	2.500
12	C	1.260	3.258	2.535
13	H	2.342	3.371	2.486
14	C	0.434	4.381	2.626
15	H	0.885	5.372	2.645
16	C	-0.960	4.243	2.689
17	H	-1.598	5.122	2.758
18	C	-1.525	2.967	2.677
19	H	-2.602	2.828	2.746
20	C	-0.710	1.829	2.582
21	C	0.941	-0.346	0.306
22	C	2.208	-0.500	-0.289
23	C	2.367	-0.476	-1.676
24	H	3.357	-0.603	-2.114
25	C	1.251	-0.282	-2.497
26	H	1.378	-0.261	-3.577
27	C	-0.014	-0.114	-1.929
28	H	-0.885	0.041	-2.562
29	C	-0.158	-0.148	-0.537
30	H	-1.146	-0.026	-0.100
31	C	-1.200	-1.833	2.494
32	C	-2.520	-1.978	3.024
33	C	-3.087	-3.257	3.161
34	H	-4.089	-3.324	3.577
35	C	-2.382	-4.390	2.772
36	H	-2.837	-5.372	2.884
37	C	-1.090	-4.271	2.233
38	H	-0.538	-5.154	1.918
39	C	-0.520	-3.011	2.100
40	H	0.475	-2.936	1.671

imine-amine (**17b**)
B3LYP/6-31+G(d')

1	O	3.397	0.658	-1.132
2	H	3.073	0.906	-0.237
3	O	-3.048	-0.904	1.930
4	H	-2.576	-0.060	1.687
5	N	1.602	0.980	0.914
6	H	1.912	0.722	1.850
7	N	-1.177	0.646	1.020
8	C	0.985	-0.182	0.225
9	H	1.606	-1.037	0.519

10	C	-0.443	-0.395	0.739
11	C	0.756	2.136	0.939
12	C	1.283	3.427	0.996
13	H	2.363	3.561	1.010
14	C	0.422	4.530	1.007
15	H	0.835	5.536	1.039
16	C	-0.966	4.339	0.955
17	H	-1.634	5.198	0.949
18	C	-1.495	3.049	0.924
19	H	-2.570	2.882	0.910
20	C	-0.639	1.936	0.927
21	C	1.072	-0.027	-1.297
22	C	2.303	0.347	-1.885
23	C	2.438	0.392	-3.279
24	H	3.401	0.684	-3.693
25	C	1.354	0.080	-4.099
26	H	1.470	0.120	-5.181
27	C	0.122	-0.269	-3.535
28	H	-0.731	-0.502	-4.168
29	C	-0.007	-0.318	-2.145
30	H	-0.965	-0.599	-1.713
31	C	-0.990	-1.740	0.940
32	C	-2.274	-1.928	1.539
33	C	-2.771	-3.228	1.742
34	H	-3.748	-3.330	2.209
35	C	-2.033	-4.336	1.346
36	H	-2.435	-5.335	1.508
37	C	-0.778	-4.175	0.735
38	H	-0.204	-5.040	0.413
39	C	-0.274	-2.895	0.541
40	H	0.690	-2.786	0.051

ene-diamine (**18a**)
B3LYP/6-31+G(d')

1	C	2.021	1.183	-1.238
2	C	1.020	1.517	-0.307
3	C	1.169	2.712	0.439
4	C	2.304	3.516	0.268
5	C	3.291	3.150	-0.646
6	C	3.150	1.982	-1.409
7	C	-0.179	0.667	-0.115
8	N	-1.408	1.410	-0.136
9	C	-2.640	0.698	-0.078
10	C	-2.640	-0.699	0.078
11	N	-1.408	-1.410	0.136

12	C	-0.179	-0.668	0.115
13	C	-3.855	-1.384	0.157
14	C	-5.071	-0.694	0.083
15	C	-5.071	0.693	-0.083
16	C	-3.856	1.383	-0.157
17	C	1.020	-1.517	0.307
18	C	2.020	-1.184	1.239
19	C	3.150	-1.982	1.410
20	C	3.291	-3.149	0.647
21	C	2.305	-3.515	-0.269
22	C	1.170	-2.712	-0.440
23	O	0.256	-3.115	-1.371
24	O	0.254	3.116	1.369
25	H	-6.007	1.242	-0.146
26	H	-3.845	2.467	-0.263
27	H	-3.844	-2.468	0.263
28	H	-6.007	-1.243	0.147
29	H	-1.404	2.122	-0.863
30	H	-1.404	-2.123	0.861
31	H	1.899	-0.278	1.829
32	H	3.911	-1.700	2.135
33	H	4.169	-3.781	0.771
34	H	2.393	-4.418	-0.868
35	H	2.390	4.420	0.867
36	H	4.168	3.782	-0.770
37	H	3.912	1.700	-2.132
38	H	1.901	0.277	-1.826
39	H	-0.563	-2.594	-1.260
40	H	-0.565	2.595	1.258

ene-diamine (**18b**)
B3LYP/6-31+G(d')

1	C	1.067	2.745	0.395
2	C	0.985	1.521	-0.302
3	C	2.063	1.177	-1.136
4	C	3.192	1.991	-1.253
5	C	3.257	3.190	-0.538
6	C	2.192	3.568	0.283
7	C	-0.215	0.652	-0.201
8	C	-0.178	-0.682	0.038
9	N	-1.383	-1.466	-0.090
10	C	-2.631	-0.774	-0.016
11	C	-2.652	0.618	-0.219
12	N	-1.448	1.281	-0.510
13	C	-3.872	1.300	-0.158
14	C	-5.066	0.608	0.090

15	C	-5.042	-0.772	0.290
16	C	-3.819	-1.457	0.240
17	C	1.028	-1.499	0.305
18	C	1.926	-1.188	1.343
19	C	3.063	-1.960	1.579
20	C	3.313	-3.081	0.775
21	C	2.429	-3.425	-0.248
22	C	1.289	-2.646	-0.485
23	O	0.482	-3.019	-1.521
24	O	-0.003	3.094	1.191
25	H	-5.961	-1.320	0.483
26	H	-3.789	-2.536	0.394
27	H	-3.884	2.378	-0.311
28	H	-6.005	1.156	0.127
29	H	-1.367	-2.255	0.552
30	H	-1.460	2.275	-0.323
31	H	2.004	0.251	-1.700
32	H	4.010	1.692	-1.905
33	H	4.129	3.836	-0.620
34	H	2.232	4.505	0.840
35	H	2.604	-4.292	-0.882
36	H	4.195	-3.694	0.950
37	H	3.743	-1.696	2.386
38	H	1.715	-0.320	1.964
39	H	0.185	3.921	1.654
40	H	-0.354	-2.515	-1.481

ene-diamine (**18c**)
B3LYP/6-31+G(d')

1	C	-0.400	4.171	2.079
2	C	-1.141	3.042	1.692
3	C	-0.505	1.849	1.349
4	C	0.904	1.777	1.395
5	C	1.637	2.903	1.773
6	C	0.991	4.104	2.109
7	N	-1.238	0.728	0.913
8	N	1.542	0.555	1.103
9	C	-0.574	-0.492	0.617
10	C	0.782	-0.565	0.672
11	C	1.575	-1.795	0.417
12	C	-1.462	-1.587	0.149
13	C	1.263	-3.008	1.056
14	C	2.007	-4.170	0.844
15	C	3.112	-4.138	-0.012
16	C	3.463	-2.941	-0.643

17	C	2.706	-1.785	-0.427
18	C	-2.607	-1.973	0.876
19	C	-3.454	-2.987	0.417
20	C	-3.178	-3.639	-0.788
21	C	-2.060	-3.263	-1.538
22	C	-1.227	-2.245	-1.072
23	O	3.031	-0.593	-1.038
24	O	-2.857	-1.315	2.062
25	H	-0.917	5.091	2.342
26	H	-2.229	3.094	1.635
27	H	2.723	2.833	1.823
28	H	1.581	4.970	2.400
29	H	-2.148	0.612	1.340
30	H	2.450	0.634	0.665
31	H	0.416	-3.025	1.737
32	H	1.732	-5.091	1.353
33	H	3.706	-5.032	-0.185
34	H	4.327	-2.903	-1.307
35	H	-4.327	-3.268	1.006
36	H	-3.842	-4.427	-1.138
37	H	-1.842	-3.751	-2.485
38	H	-0.368	-1.936	-1.663
39	H	3.800	-0.712	-1.612
40	H	-3.646	-1.680	2.485

5	H	0.446	-1.468	0.093
6	H	-0.446	1.468	-0.095
7	H	-2.507	0.431	0.523
8	H	-1.976	-1.064	0.063
9	H	1.976	1.064	-0.065
10	H	2.507	-0.432	-0.523

C₂H₆N₂ (**20a-E**)
B3LYP/6-311++G(d,p)

1	C	-0.378	0.330	0.000
2	C	1.125	0.507	0.000
3	N	-0.920	-0.817	0.000
4	N	1.938	-0.697	0.000
5	H	-0.953	1.268	0.000
6	H	1.389	1.122	0.870
7	H	1.390	1.122	-0.870
8	H	-1.938	-0.747	0.000
9	H	1.707	-1.268	-0.808
10	H	1.707	-1.268	0.807

DFT structures and coordinates: Figure 7

C₂H₆N₂ (**19-Z**)
B3LYP/6-311++G(d,p)

1	C	-0.669	0.494	0.015
2	C	0.669	0.494	-0.017
3	N	-1.434	-0.694	0.069
4	N	1.433	-0.694	-0.071
5	H	-1.215	1.427	0.061
6	H	1.214	1.428	-0.063
7	H	-1.075	-1.428	-0.532
8	H	-2.416	-0.551	-0.115
9	H	2.416	-0.550	0.112
10	H	1.076	-1.427	0.532

C₂H₆N₂ (**20b-E**)
B3LYP/6-311++G(d,p)

1	C	-0.624	-0.276	-0.510
2	C	0.265	0.214	0.602
3	N	-1.000	0.494	-1.448
4	N	1.400	-0.700	0.771
5	H	-0.900	-1.337	-0.443
6	H	-0.319	0.194	1.530
7	H	0.532	1.259	0.400
8	H	-1.603	0.000	-2.108
9	H	1.882	-0.533	1.646
10	H	2.072	-0.587	0.021

C₂H₆N₂ (**19-E**)
B3LYP/6-311++G(d,p)

1	C	0.544	-0.387	0.028
2	C	-0.545	0.387	-0.030
3	N	-1.883	-0.068	-0.100
4	N	1.882	0.068	0.098

C₂H₆N₂ (**20a-Z**)
B3LYP/6-311++G(d,p)

1	C	-0.928	-0.213	0.000
2	C	0.081	0.927	0.000
3	N	-0.663	-1.450	0.000
4	N	1.462	0.447	0.000
5	H	-1.978	0.097	0.000

6	H	-0.126	1.559	0.873
7	H	-0.126	1.559	-0.873
8	H	0.360	-1.559	0.000
9	H	1.978	0.734	0.820
10	H	1.978	0.734	-0.820

C₂H₆N₂ (**20b-Z**)
B3LYP/6-311++G(d,p)

1	C	0.856	0.480	0.000
2	C	-0.652	0.682	0.000
3	N	1.500	-0.611	0.000
4	N	-1.500	-0.496	0.000
5	H	1.438	1.408	0.000
6	H	-0.904	1.300	-0.871
7	H	-0.904	1.300	0.871
8	H	0.854	-1.408	0.000
9	H	-1.373	-1.072	0.824
10	H	-1.373	-1.072	-0.825

s-trans-hydroxy-acetaldehyde (**21**)
B3LYP/6-311++G(d,p)

1	C	-0.115	0.493	0.000
2	C	-0.379	-1.000	0.000
3	O	-1.485	-1.477	0.000
4	O	1.291	0.687	0.000
5	H	-0.598	0.922	0.888
6	H	-0.598	0.922	-0.888
7	H	0.537	-1.629	0.000
8	H	1.485	1.629	0.000

E-ethylene-1,2-diol (**22**)
B3LYP/6-311++G(d,p)

1	C	-0.547	-0.376	0.029
2	C	0.547	0.376	-0.029
3	O	1.800	-0.203	-0.048
4	O	-1.800	0.203	0.048
5	H	-0.492	-1.458	0.104
6	H	0.492	1.458	-0.104
7	H	2.435	0.400	0.345
8	H	-2.435	-0.400	-0.344

Summary of computationally studied species

All reported energies include zero point energy and use pure d orbitals. E (hartrees), enthalpy (hartrees), entropy (cal/molK), and Gibbs free energy (hartrees) are taken directly from the file output. The Gibbs free energy values are calculated for $T = 298.150$ K.

species	structure	E (hartrees)	relative E (kcal/mol)	enthalpy (hartrees)	entropy (cal/molK)	Gibbs free energy (hartrees)	Gibbs free energy (kcal/mol)	relative Gibbs free energy (kcal/mol)
Figure 5 B3LYP/6-31+G(d')								
2		-690.938538	0.0000	-690.924363	117.903	-690.980383	-433596.4092	0.0000
3-Z		-690.920309	11.4389	-690.906023	115.954	-690.961117	-433584.3196	12.0896
3-E		-690.916364	13.9144	-690.902136	115.257	-690.956898	-433581.6721	14.7370
Figure 6 B3LYP/6-31+G(d')								
13-E		-1113.104755	0.0000	-1113.080797	166.482	-1113.159898	-698517.8544	0.0000
13-Z		-1113.103297	0.9149	-1113.079111	168.342	-1113.159096	-698517.3512	0.5033
14-E		-1113.102505	1.4119	-1113.07852	169.032	-1113.158833	-698517.1861	0.6683
14-Z		-1113.097936	4.2790	-1113.073869	168.976	-1113.154155	-698514.2506	3.6038

species	structure	E (hartrees)	relative E (kcal/mol)	Enthalpy (hartrees)	entropy (cal/molK)	Gibbs free energy (hartrees)	Gibbs free energy (kcal/mol)	relative Gibbs free energy (kcal/mol)
Figure 6 B3LYP/6-31+G(d')								
17a		-1031.407052	0.0000	-1031.387677	140.573	-1031.454468	-647246.9618	0.0000
17b		-1031.405052	1.2550	-1031.386148	138.025	-1031.451728	-647245.2424	1.7194
18a		-1031.392923	8.8661	-1031.373359	140.749	-1031.440233	-647238.0292	8.9326
18b		-1031.388369	11.7238	-1031.368461	142.464	-1031.43615	-647235.4671	11.4947
18c		-1031.38049	16.6679	-1031.360081	145.444	-1031.429186	-647231.0971	15.8647
Figure 7 B3LYP/6-311++G(d,p)								
19-Z		-189.280873	0.0000	-189.274624	71.056	-189.308385	-118792.7154	0.0000
20a-E		-189.277648	2.0237	-189.271732	69.700	-189.304849	-118790.4965	2.2189
20b-E		-189.275962	3.0817	-189.270039	69.879	-189.303241	-118789.4875	3.2279
20a-Z		-189.276711	2.6117	-189.271445	66.916	-189.303239	-118789.4862	3.2292
20b-Z		-189.276048	3.0277	-189.270272	68.799	-189.30296	-118789.3111	3.4042
19e		-189.275856	3.1482	-189.269621	70.015	-189.302888	-118789.2659	3.4494
Figure 7 B3LYP/6-311++G(d,p)								
21		-229.055771	0.0000	-229.049822	70.493	-229.083316	-143751.8425	0.0000
22		-229.040043	9.8695	-229.033878	70.261	-229.067262	-143741.7685	10.0740

**X-Ray Structure Data for *E*-1,2,*N,N'*-tetraphenylethylene-1,2-diamine
13-*E*
(SM18) C₂₆H₂₂N₂**

Labeled view with 50% probability ellipsoids

Table 1. Crystal data and structure refinement for *E*-1,2,*N,N'*-tetraphenylethylene-1,2-diamine (SM18): C₂₆H₂₂N₂.

Identification code	SM18	
Empirical formula	C ₂₆ H ₂₂ N ₂	
Formula weight	362.47	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.091(7) Å	α = 90°
	b = 8.924(5) Å	β = 101.359(11)°
	c = 19.781(12) Å	γ = 90°
Volume	1919.4(19) Å ³	
Z	4	
Density (calculated)	1.254 Mg/m ³	
Absorption coefficient	0.073 mm ⁻¹	
F(000)	768	
Crystal size	0.50 × 0.17 × 0.05 mm ³	
Theta range for data collection	1.87 to 25.00°	
Index ranges	-13 ≤ h ≤ 13, -10 ≤ k ≤ 10, -23 ≤ l ≤ 20	
Reflections collected	13175	
Independent reflections	3333 [R(int) = 0.0389]	
Completeness to theta = 25.00°	98.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3333 / 0 / 225	
Goodness-of-fit on F ²	1.008	
Final R indices [I > 2σ(I)]	R1 = 0.0574, wR2 = 0.1340	
R indices (all data)	R1 = 0.0850, wR2 = 0.1732	
Largest diff. peak and hole	0.337 and -0.239 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *E*-1,2,*N,N'*-tetraphenylethylene-1,2-diamine (SM18): $\text{C}_{26}\text{H}_{22}\text{N}_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3830(2)	-1243(2)	10126(1)	32(1)
N(2)	2574(2)	2280(2)	9354(1)	32(1)
C(1)	3039(2)	13(2)	9992(1)	31(1)
C(2)	2881(2)	747(3)	9381(1)	30(1)
C(3)	3469(2)	-2630(2)	10352(1)	31(1)
C(4)	4357(2)	-3736(3)	10550(1)	33(1)
C(5)	4029(2)	-5112(3)	10780(1)	39(1)
C(6)	2816(2)	-5406(3)	10819(1)	40(1)
C(7)	1939(2)	-4315(3)	10620(1)	39(1)
C(8)	2247(2)	-2938(3)	10382(1)	34(1)
C(9)	2535(2)	552(2)	10589(1)	31(1)
C(10)	3235(2)	475(3)	11255(1)	35(1)
C(11)	2753(2)	922(3)	11815(1)	40(1)
C(12)	1550(2)	1433(3)	11720(1)	40(1)
C(13)	830(2)	1492(3)	11060(1)	39(1)
C(14)	1317(2)	1063(3)	10498(1)	34(1)
C(15)	1574(2)	2908(3)	8886(1)	32(1)
C(16)	615(2)	2040(3)	8525(1)	33(1)
C(17)	-359(2)	2720(3)	8087(1)	37(1)
C(18)	-384(2)	4259(3)	7992(1)	38(1)
C(19)	574(2)	5115(3)	8349(1)	39(1)
C(20)	1546(2)	4455(3)	8794(1)	34(1)
C(21)	3184(2)	98(3)	8741(1)	31(1)
C(22)	3048(2)	-1431(3)	8595(1)	34(1)
C(23)	3338(2)	-2028(3)	8004(1)	38(1)
C(24)	3734(2)	-1114(3)	7526(1)	40(1)
C(25)	3844(2)	413(3)	7651(1)	36(1)
C(26)	3583(2)	1003(3)	8254(1)	33(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for *E*-1,2,*N,N'*-tetraphenylethylene-1,2-diamine (SM18): $\text{C}_{26}\text{H}_{22}\text{N}_2$.

N(1)-C(3)	1.400(3)
N(1)-C(1)	1.416(3)
N(2)-C(2)	1.408(3)
N(2)-C(15)	1.412(3)
C(1)-C(2)	1.355(3)
C(1)-C(9)	1.484(3)
C(2)-C(21)	1.489(3)
C(3)-C(4)	1.395(3)
C(3)-C(8)	1.396(3)
C(4)-C(5)	1.383(3)
C(5)-C(6)	1.388(4)
C(6)-C(7)	1.378(4)
C(7)-C(8)	1.383(4)
C(9)-C(10)	1.393(3)
C(9)-C(14)	1.403(3)
C(10)-C(11)	1.379(4)
C(11)-C(12)	1.387(4)
C(12)-C(13)	1.390(4)
C(13)-C(14)	1.381(3)
C(15)-C(20)	1.393(3)
C(15)-C(16)	1.394(3)
C(16)-C(17)	1.384(3)
C(17)-C(18)	1.385(4)
C(18)-C(19)	1.385(4)
C(19)-C(20)	1.381(4)
C(21)-C(26)	1.394(3)

C(21)-C(22)	1.397(3)
C(22)-C(23)	1.379(4)
C(23)-C(24)	1.383(4)
C(24)-C(25)	1.386(4)
C(25)-C(26)	1.386(4)
C(3)-N(1)-C(1)	123.66(19)
C(2)-N(2)-C(15)	124.25(19)
C(2)-C(1)-N(1)	121.1(2)
C(2)-C(1)-C(9)	123.4(2)
N(1)-C(1)-C(9)	115.0(2)
C(1)-C(2)-N(2)	119.4(2)
C(1)-C(2)-C(21)	124.0(2)
N(2)-C(2)-C(21)	116.0(2)
C(4)-C(3)-C(8)	119.1(2)
C(4)-C(3)-N(1)	119.0(2)
C(8)-C(3)-N(1)	121.9(2)
C(5)-C(4)-C(3)	120.2(2)
C(4)-C(5)-C(6)	120.5(2)
C(7)-C(6)-C(5)	119.2(2)
C(6)-C(7)-C(8)	121.2(2)
C(7)-C(8)-C(3)	119.8(2)
C(10)-C(9)-C(14)	118.7(2)
C(10)-C(9)-C(1)	120.7(2)
C(14)-C(9)-C(1)	120.5(2)
C(11)-C(10)-C(9)	120.8(2)
C(10)-C(11)-C(12)	120.1(2)
C(11)-C(12)-C(13)	119.9(2)
C(14)-C(13)-C(12)	120.1(2)
C(13)-C(14)-C(9)	120.4(2)
C(20)-C(15)-C(16)	119.2(2)
C(20)-C(15)-N(2)	118.3(2)
C(16)-C(15)-N(2)	122.5(2)
C(17)-C(16)-C(15)	120.0(2)
C(16)-C(17)-C(18)	120.8(2)
C(19)-C(18)-C(17)	119.0(2)
C(20)-C(19)-C(18)	120.9(2)
C(19)-C(20)-C(15)	120.1(2)
C(26)-C(21)-C(22)	117.3(2)
C(26)-C(21)-C(2)	121.1(2)
C(22)-C(21)-C(2)	121.5(2)
C(23)-C(22)-C(21)	121.2(2)
C(22)-C(23)-C(24)	120.6(2)
C(23)-C(24)-C(25)	119.1(2)
C(26)-C(25)-C(24)	120.1(2)
C(25)-C(26)-C(21)	121.5(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *E*-1,2,*N,N'*-tetraphenylethylene-1,2-diamine (SM18): $\text{C}_{26}\text{H}_{22}\text{N}_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	30(1)	31(1)	36(1)	2(1)	8(1)	3(1)
N(2)	36(1)	28(1)	31(1)	-2(1)	3(1)	-1(1)
C(1)	28(1)	27(1)	37(1)	-2(1)	7(1)	-1(1)
C(2)	27(1)	28(1)	34(1)	-1(1)	4(1)	-2(1)
C(3)	35(1)	28(1)	29(1)	-1(1)	6(1)	0(1)
C(4)	34(1)	31(1)	34(1)	-1(1)	6(1)	1(1)
C(5)	51(2)	31(1)	35(2)	-2(1)	4(1)	3(1)
C(6)	56(2)	32(1)	34(1)	-1(1)	11(1)	-9(1)
C(7)	43(2)	40(1)	37(2)	-6(1)	12(1)	-11(1)
C(8)	32(1)	34(1)	35(1)	-4(1)	7(1)	-1(1)
C(9)	31(1)	26(1)	35(1)	0(1)	9(1)	-3(1)
C(10)	36(1)	33(1)	36(1)	2(1)	6(1)	3(1)

C(11)	51(2)	34(1)	33(1)	0(1)	7(1)	0(1)
C(12)	50(2)	33(1)	42(2)	-3(1)	20(1)	-4(1)
C(13)	32(1)	34(1)	52(2)	-3(1)	13(1)	-4(1)
C(14)	33(1)	33(1)	36(1)	-1(1)	8(1)	-5(1)
C(15)	33(1)	31(1)	31(1)	2(1)	7(1)	1(1)
C(16)	34(1)	29(1)	38(1)	-1(1)	9(1)	0(1)
C(17)	32(1)	41(1)	38(2)	-4(1)	7(1)	-1(1)
C(18)	35(1)	44(2)	35(1)	1(1)	9(1)	9(1)
C(19)	46(2)	32(1)	42(2)	5(1)	15(1)	7(1)
C(20)	37(1)	31(1)	36(1)	-3(1)	10(1)	0(1)
C(21)	24(1)	36(1)	33(1)	2(1)	1(1)	2(1)
C(22)	34(1)	35(1)	32(1)	4(1)	1(1)	2(1)
C(23)	36(1)	34(1)	40(2)	-3(1)	0(1)	5(1)
C(24)	36(1)	51(2)	31(1)	-3(1)	3(1)	7(1)
C(25)	29(1)	43(1)	34(1)	3(1)	4(1)	0(1)
C(26)	28(1)	35(1)	33(1)	2(1)	1(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *E*-1,2,*N,N'*-tetraphenylethylene-1,2-diamine (SM18): $\text{C}_{26}\text{H}_{22}\text{N}_2$.

	x	y	z	U(eq)
H(1)	4419	-1412	9872	44(8)
H(2)	2784	2723	9756	38(7)
H(4A)	5191	-3543	10528	40
H(5A)	4638	-5862	10911	47
H(6A)	2594	-6348	10982	48
H(7A)	1108	-4513	10645	47
H(8A)	1629	-2203	10240	41
H(10A)	4055	111	11325	42
H(11A)	3245	879	12265	47
H(12A)	1218	1741	12105	48
H(13A)	3	1829	10995	46
H(14A)	824	1114	10048	41
H(16A)	629	982	8579	40
H(17A)	-1018	2124	7848	45
H(18A)	-1049	4719	7686	45
H(19A)	564	6171	8287	47
H(20A)	2195	5058	9037	41
H(22A)	2751	-2072	8909	41
H(23A)	3266	-3077	7924	45
H(24A)	3927	-1527	7118	48
H(25A)	4099	1055	7323	43
H(26A)	3679	2049	8338	39

**X-Ray Structure Data for *E*-1,2,-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine
13-Me₂-*E*
(SM81) C₂₈H₂₆N₂**

Labeled view with 50% probability ellipsoids

Table 6. Crystal data and structure refinement for *E*-1,2,-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (SM81): C₂₈H₂₆N₂.

Identification code	sm81a	
Empirical formula	C ₂₈ H ₂₆ N ₂	
Formula weight	390.51	
Temperature	110(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Fdd2	
Unit cell dimensions	a = 16.5867(17) Å	α = 90°
	b = 44.319(6) Å	β = 90°
	c = 5.7826(6) Å	γ = 90°
Volume	4250.8(8) Å ³	
Z	8	
Density (calculated)	1.220 Mg/m ³	
Absorption coefficient	0.0542 mm ⁻¹	
F(000)	1664	
Crystal size	0.06 x 0.02 x 0.02 mm ³	
Theta range for data collection	3.99 to 58.93°	
Index ranges	-18 ≤ h ≤ 18, -47 ≤ k ≤ 48, -6 ≤ l ≤ 6	
Reflections collected	9561	
Independent reflections	1534 [R(int) = 0.0931]	
Completeness to theta = 58.93°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1534 / 1 / 138	
Goodness-of-fit on F ²	0.000	
Final R indices [I > 2σ(I)]	R1 = 0.0430, wR2 = 0.1024	
R indices (all data)	R1 = 0.0628, wR2 = 0.1172	
Largest diff. peak and hole	0.250 and -0.261 Å ⁻³	

Table 7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *E*-1,2-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (SM81): $\text{C}_{28}\text{H}_{26}\text{N}_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4522(1)	374(1)	7885(4)	24(1)
C(1)	4389(2)	615(1)	6335(5)	22(1)
C(2)	4752(2)	625(1)	4164(5)	26(1)
C(3)	4642(2)	874(1)	2739(5)	27(1)
C(4)	4165(2)	1118(1)	3401(5)	26(1)
C(5)	3774(2)	1098(1)	5534(5)	31(1)
C(6)	3886(2)	854(1)	6980(5)	27(1)
C(7)	5102(2)	149(1)	7471(5)	24(1)
C(8)	5957(2)	253(1)	7399(5)	23(1)
C(9)	6486(2)	157(1)	5671(5)	25(1)
C(10)	7280(2)	256(1)	5618(5)	29(1)
C(11)	7560(2)	453(1)	7308(5)	29(1)
C(12)	7046(2)	550(1)	9031(5)	29(1)
C(13)	6244(2)	453(1)	9063(5)	25(1)
C(14)	4090(2)	1392(1)	1884(5)	36(1)

Table 8. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for *E*-1,2-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (SM81): $\text{C}_{28}\text{H}_{26}\text{N}_2$.

N(1)-C(7)	1.407(4)
N(1)-C(1)	1.412(4)
C(1)-C(2)	1.393(4)
C(1)-C(6)	1.399(4)
C(2)-C(3)	1.387(4)
C(3)-C(4)	1.396(4)
C(4)-C(5)	1.396(4)
C(4)-C(14)	1.502(4)
C(5)-C(6)	1.377(4)
C(7)-C(7)A	1.361(6)
C(7)-C(8)	1.491(4)
C(8)-C(13)	1.394(4)
C(8)-C(9)	1.397(4)
C(9)-C(10)	1.388(4)
C(10)-C(11)	1.391(4)
C(11)-C(12)	1.381(4)
C(12)-C(13)	1.397(4)
C(7)-N(1)-C(1)	122.5(2)
C(2)-C(1)-C(6)	118.3(3)
C(2)-C(1)-N(1)	121.8(3)
C(6)-C(1)-N(1)	119.9(2)
C(3)-C(2)-C(1)	120.2(3)
C(2)-C(3)-C(4)	121.9(3)
C(5)-C(4)-C(3)	117.0(3)
C(5)-C(4)-C(14)	122.0(3)
C(3)-C(4)-C(14)	121.0(3)
C(6)-C(5)-C(4)	121.7(3)
C(5)-C(6)-C(1)	120.7(3)
C(7)A-C(7)-N(1)	121.1(3)
C(7)A-C(7)-C(8)	122.4(3)
N(1)-C(7)-C(8)	115.8(3)
C(13)-C(8)-C(9)	118.2(2)
C(13)-C(8)-C(7)	120.2(3)
C(9)-C(8)-C(7)	121.6(3)
C(10)-C(9)-C(8)	121.1(3)
C(9)-C(10)-C(11)	120.0(3)

C(12)-C(11)-C(10)	119.8(3)
C(11)-C(12)-C(13)	120.1(3)
C(8)-C(13)-C(12)	120.8(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,z

Table 9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *E*-1,2-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (SM81): $\text{C}_{28}\text{H}_{26}\text{N}_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	18(1)	28(2)	27(1)	0(1)	3(1)	0(1)
C(1)	18(1)	28(2)	21(1)	1(2)	-2(1)	-2(1)
C(2)	22(2)	34(3)	21(2)	-3(2)	-1(1)	5(2)
C(3)	25(2)	36(2)	21(2)	1(2)	1(1)	-3(2)
C(4)	25(2)	29(2)	25(2)	-2(2)	-4(1)	2(1)
C(5)	28(2)	36(3)	29(2)	-6(2)	0(1)	6(2)
C(6)	23(2)	35(2)	24(2)	-3(2)	2(1)	3(2)
C(7)	18(2)	31(2)	22(1)	0(1)	3(1)	0(1)
C(8)	20(1)	25(2)	25(2)	3(2)	2(1)	2(1)
C(9)	24(2)	32(2)	20(2)	-1(2)	-1(1)	-2(1)
C(10)	21(2)	43(3)	25(2)	2(2)	5(1)	3(2)
C(11)	19(1)	36(2)	33(2)	3(2)	-1(1)	-2(1)
C(12)	29(2)	32(2)	28(2)	-2(2)	-2(1)	-2(1)
C(13)	23(2)	28(2)	23(2)	-1(2)	1(1)	0(1)
C(14)	41(2)	36(3)	31(2)	3(2)	-4(1)	5(2)

Table 10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *E*-1,2-diphenyl-*N,N'*-di-(*p*-methylphenyl)-ethylene-1,2-diamine (SM81): $\text{C}_{28}\text{H}_{26}\text{N}_2$.

	x	y	z	U(eq)
H(1)	4037	306	8212	29
H(2A)	5076	461	3658	31
H(3A)	4899	877	1271	33
H(5A)	3422	1255	5998	37
H(6A)	3619	849	8433	33
H(9A)	6300	21	4513	30
H(10A)	7632	189	4427	35
H(11A)	8103	520	7277	35
H(12A)	7237	682	10198	35
H(13A)	5890	525	10233	30
H(14A)	4617	1490	1747	54
H(14B)	3703	1533	2569	54
H(14C)	3902	1331	347	54

X-Ray Structure Data for 2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline.

17a
(SM11) C₂₀H₁₆N₂O₂

Labeled view with 50% probability ellipsoids

Table 11. Crystal data and structure refinement for 2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline (SM11): C₂₀H₁₆N₂O₂.

Identification code	SM11	
Empirical formula	C ₂₀ H ₁₆ N ₂ O ₂	
Formula weight	316.35	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.708(2) Å	α = 90°
	b = 15.970(4) Å	β = 115.496(3)°
	c = 11.254(3) Å	γ = 90°
Volume	1574.9(6) Å ³	
Z	4	
Density (calculated)	1.334 Mg/m ³	
Absorption coefficient	0.087 mm ⁻¹	
F(000)	664	
Crystal size	0.2 x 0.2 x 0.05 mm ³	
Theta range for data collection	2.33 to 27.52°	
Index ranges	-12 ≤ h ≤ 12, -19 ≤ k ≤ 10, -7 ≤ l ≤ 14	
Reflections collected	9737	
Independent reflections	3553 [R(int) = 0.0547]	
Completeness to theta = 25.00°	97.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3553 / 0 / 229	
Goodness-of-fit on F ²	1.056	
Final R indices [I > 2σ(I)]	R1 = 0.0557, wR2 = 0.1015	
R indices (all data)	R1 = 0.1188, wR2 = 0.1140	
Largest diff. peak and hole	0.319 and -0.223 e.Å ⁻³	

Table 12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline (SM11): $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4290(2)	533(1)	6433(2)	37(1)
O(2)	11669(2)	290(1)	6698(2)	34(1)
N(1)	6403(2)	1295(1)	5439(2)	32(1)
N(2)	9494(2)	1143(1)	6629(2)	29(1)
C(1)	7037(2)	573(1)	6323(2)	26(1)
C(2)	8667(2)	480(1)	6504(2)	25(1)
C(3)	7259(3)	2029(2)	5816(2)	30(1)
C(4)	6611(3)	2822(2)	5492(2)	36(1)
C(5)	7541(3)	3512(2)	5860(2)	42(1)
C(6)	9110(3)	3439(2)	6555(3)	40(1)
C(7)	9750(3)	2650(2)	6824(2)	38(1)
C(8)	8832(3)	1941(1)	6456(2)	29(1)
C(9)	6946(2)	676(1)	7633(2)	25(1)
C(10)	5500(2)	656(1)	7631(2)	28(1)
C(11)	5342(3)	761(1)	8788(2)	32(1)
C(12)	6613(3)	886(1)	9957(2)	36(1)
C(13)	8052(3)	911(1)	9991(2)	35(1)
C(14)	8202(3)	805(1)	8823(2)	30(1)
C(15)	9352(2)	-347(1)	6547(2)	25(1)
C(16)	10817(2)	-412(1)	6592(2)	29(1)
C(17)	11419(2)	-1189(2)	6539(2)	33(1)
C(18)	10610(3)	-1911(2)	6475(2)	35(1)
C(19)	9179(3)	-1868(2)	6469(2)	36(1)
C(20)	8554(2)	-1089(1)	6495(2)	31(1)

Table 13. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for 2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline (SM11): $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_2$.

O(1)-C(10)	1.368(2)
O(2)-C(16)	1.368(2)
N(1)-C(3)	1.393(3)
N(1)-C(1)	1.473(3)
N(2)-C(2)	1.299(2)
N(2)-C(8)	1.403(3)
C(1)-C(2)	1.513(3)
C(1)-C(9)	1.523(3)
C(2)-C(15)	1.470(3)
C(3)-C(8)	1.387(3)
C(3)-C(4)	1.391(3)
C(4)-C(5)	1.370(3)
C(5)-C(6)	1.386(3)
C(6)-C(7)	1.379(3)
C(7)-C(8)	1.390(3)
C(9)-C(14)	1.385(3)
C(9)-C(10)	1.403(3)
C(10)-C(11)	1.385(3)
C(11)-C(12)	1.377(3)
C(12)-C(13)	1.382(3)
C(13)-C(14)	1.393(3)
C(15)-C(20)	1.402(3)
C(15)-C(16)	1.405(3)
C(16)-C(17)	1.383(3)
C(17)-C(18)	1.379(3)
C(18)-C(19)	1.388(3)
C(19)-C(20)	1.391(3)
C(3)-N(1)-C(1)	115.64(19)
C(2)-N(2)-C(8)	119.98(19)

N(1)-C(1)-C(2)	106.03(17)
N(1)-C(1)-C(9)	112.73(18)
C(2)-C(1)-C(9)	111.94(18)
N(2)-C(2)-C(15)	118.62(19)
N(2)-C(2)-C(1)	119.8(2)
C(15)-C(2)-C(1)	121.58(18)
C(8)-C(3)-C(4)	120.1(2)
C(8)-C(3)-N(1)	116.8(2)
C(4)-C(3)-N(1)	122.9(2)
C(5)-C(4)-C(3)	119.2(2)
C(4)-C(5)-C(6)	121.6(2)
C(7)-C(6)-C(5)	118.8(2)
C(6)-C(7)-C(8)	120.6(2)
C(3)-C(8)-C(7)	119.5(2)
C(3)-C(8)-N(2)	120.1(2)
C(7)-C(8)-N(2)	120.2(2)
C(14)-C(9)-C(10)	117.9(2)
C(14)-C(9)-C(1)	123.96(19)
C(10)-C(9)-C(1)	118.09(19)
O(1)-C(10)-C(11)	123.2(2)
O(1)-C(10)-C(9)	116.1(2)
C(11)-C(10)-C(9)	120.7(2)
C(12)-C(11)-C(10)	120.0(2)
C(11)-C(12)-C(13)	120.6(2)
C(12)-C(13)-C(14)	119.0(2)
C(9)-C(14)-C(13)	121.7(2)
C(20)-C(15)-C(16)	118.1(2)
C(20)-C(15)-C(2)	121.6(2)
C(16)-C(15)-C(2)	120.25(19)
O(2)-C(16)-C(17)	119.3(2)
O(2)-C(16)-C(15)	120.4(2)
C(17)-C(16)-C(15)	120.3(2)
C(18)-C(17)-C(16)	120.7(2)
C(17)-C(18)-C(19)	120.4(2)
C(18)-C(19)-C(20)	119.3(2)
C(19)-C(20)-C(15)	121.2(2)

Table 14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline (SM11): $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	23(1)	57(1)	33(1)	-6(1)	14(1)	-5(1)
O(2)	28(1)	39(1)	38(1)	0(1)	17(1)	-3(1)
N(1)	25(1)	36(1)	33(1)	3(1)	10(1)	1(1)
N(2)	29(1)	32(1)	31(1)	1(1)	16(1)	-1(1)
C(1)	23(1)	28(1)	27(1)	-1(1)	9(1)	-3(1)
C(2)	25(1)	30(1)	18(1)	-3(1)	9(1)	-5(1)
C(3)	35(1)	30(2)	31(2)	2(1)	19(1)	2(1)
C(4)	36(2)	38(2)	36(2)	4(1)	17(1)	7(1)
C(5)	55(2)	30(2)	46(2)	2(1)	26(2)	3(1)
C(6)	43(2)	28(2)	52(2)	-4(1)	24(2)	-7(1)
C(7)	35(2)	38(2)	42(2)	-5(1)	19(1)	-6(1)
C(8)	33(1)	30(1)	27(2)	2(1)	15(1)	1(1)
C(9)	28(1)	23(1)	25(1)	-1(1)	12(1)	-1(1)
C(10)	23(1)	30(1)	29(2)	-1(1)	11(1)	-3(1)
C(11)	27(1)	38(2)	34(2)	-2(1)	16(1)	-4(1)
C(12)	41(2)	41(2)	31(2)	-2(1)	19(1)	-4(1)
C(13)	33(1)	41(2)	26(2)	-4(1)	10(1)	-5(1)
C(14)	29(1)	30(1)	32(2)	-1(1)	14(1)	-3(1)
C(15)	21(1)	33(1)	21(1)	1(1)	9(1)	2(1)
C(16)	29(1)	34(2)	23(1)	-1(1)	11(1)	-2(1)

C(17)	28(1)	41(2)	31(2)	2(1)	15(1)	9(1)
C(18)	40(2)	31(2)	35(2)	-3(1)	16(1)	6(1)
C(19)	38(2)	32(2)	37(2)	2(1)	16(1)	0(1)
C(20)	32(1)	33(2)	29(2)	-1(1)	13(1)	2(1)

Table 15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2,3-di-(2-hydroxyphenyl)-1,2-dihydroquinoxaline (SM11): $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_2$.

	x	y	z	U(eq)
H(1O)	3400(30)	488(16)	6560(30)	79(10)
H(2O)	10880(30)	954(15)	6680(20)	68(8)
H(1N)	5400(30)	1360(13)	5160(20)	49(8)
H(1C)	6454	60	5875	32
H(4A)	5537	2885	5020	43
H(5A)	7099	4053	5633	50
H(6A)	9734	3924	6842	48
H(7A)	10828	2592	7264	45
H(11A)	4358	746	8775	38
H(12A)	6499	956	10748	44
H(13A)	8927	1000	10799	42
H(14A)	9190	822	8844	36
H(17A)	12400	-1226	6547	39
H(18A)	11034	-2440	6434	42
H(19A)	8633	-2366	6447	43
H(20A)	7569	-1058	6478	37

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