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The Bethe-Salpeter Formalism with Polarisable Continuum Embedding: Reconciling Linear-Response and State-Specific Features: ESI

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S1 Cartesian coordinates

S1.1 Acrolein

6	-0.150509	-0.742320	-0.000000
8	-1.221242	-1.319646	-0.000000
1	0.802823	-1.302877	0.000000
6	-0.000000	0.724345	0.000000
6	1.218487	1.276311	0.000000
1	-0.905397	1.314305	-0.000000
1	1.363815	2.344937	0.000000
1	2.100824	0.650783	0.000000

S1.2 Indigo

6	-0.588979	2.930950	0.000000
6	0.813957	2.793967	0.000000
6	1.639213	3.915686	0.000000
6	1.027288	5.169382	0.000000
6	-0.369194	5.310246	0.000000
6	-1.190632	4.186090	0.000000
6	-1.161448	1.574198	0.000000
6	0.022774	0.682297	0.000000
1	2.716133	3.822424	0.000000
1	1.648545	6.053968	0.000000
1	-0.803712	6.298973	0.000000
1	-2.268631	4.267593	0.000000
1	2.083732	1.042213	0.000000
6	-0.022774	-0.682297	0.000000
6	1.161448	-1.574198	0.000000
6	0.588979	-2.930950	0.000000
6	-0.813957	-2.793967	0.000000
1	-2.083732	-1.042213	0.000000
6	1.190632	-4.186090	0.000000
6	-1.639213	-3.915686	0.000000
6	0.369194	-5.310246	0.000000
1	2.268631	-4.267593	0.000000
6	-1.027288	-5.169382	0.000000
1	-2.716133	-3.822424	0.000000
1	0.803712	-6.298973	0.000000
1	-1.648545	-6.053968	0.000000
8	-2.335875	1.199345	0.000000
8	2.335875	-1.199345	0.000000
7	1.161448	1.448720	0.000000
7	-1.161448	-1.448720	0.000000

S1.3 *para*nitroaniline

6	0.003256	1.362299	1.206029
6	0.003256	1.362299	-1.206029
6	0.003256	-0.026210	-1.212800
6	0.003326	-0.704029	-0.000000
6	0.003256	-0.026210	1.212800
1	0.007978	1.900133	-2.144629
1	0.002552	-0.585344	-2.134454
1	0.002552	-0.585344	2.134454
1	0.007978	1.900133	2.144629
7	0.000852	-2.167773	-0.000000
8	-0.000237	-2.739317	1.093615
8	-0.000237	-2.739317	-1.093615
7	0.070018	3.470230	0.000000
1	-0.302755	3.901738	-0.829058
1	-0.302755	3.901738	0.829058
6	-0.000990	2.078321	0.000000

S1.4 *para*nitroaniline (perp)

6	0.000000	1.205238	1.357916
6	-0.000000	-1.205238	1.357916
6	-0.000000	-1.217403	-0.034182
6	0.000000	-0.000000	-0.703823
6	0.000000	1.217403	-0.034182
1	-0.000000	-2.131519	1.913615
1	-0.000000	-2.135586	-0.598912
1	0.000000	2.135586	-0.598912
1	0.000000	2.131519	1.913615
7	0.000000	-0.000000	-2.174543
8	0.000000	1.093909	-2.743861
8	-0.000000	-1.093909	-2.743861
7	0.000000	0.000000	3.485857
1	-0.855647	0.000000	3.997970
1	0.855647	-0.000000	3.997970
6	0.000000	0.000000	2.072561

S1.5 benzene-TCNE (from Ref. 1)

S1.6 4-nitropyridine *N*-oxide

6	0.000000	1.188108	1.401430
6	-0.000000	-1.188108	1.401430
6	0.000000	-1.205316	0.027020
6	0.000000	-0.000000	-0.668649
6	0.000000	1.205316	0.027020
1	0.000000	-2.062566	2.029800
1	0.000000	-2.142516	-0.505527
1	0.000000	2.142516	-0.505527
1	0.000000	2.062566	2.029800
7	0.000000	-0.000000	-2.123036
8	0.000000	1.097128	-2.690242
8	-0.000000	-1.097128	-2.690242
7	-0.000000	0.000000	2.111226
8	-0.000000	0.000000	3.368562

References

1 T. Stein, L. Kronik and R. Baer, *J. Am. Chem. Soc.*, 2009, **131**, 2818–2820.