Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Investigation of the metastable structures of polyiodide in acetonitrile studied using global reaction route mapping and reference interaction site model self-consistent field explicitly including constrained spatial electron density distribution

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Contents:

1. Cartesian Coordinates (unit: Å)

Gas Phase

EQ0

0.28530201	0.27356431	0.27551079
-0.06863821	-0.06244230	3.44953311
-0.43676483	-0.40974738	6.25152332
3.45900246	-0.06909175	-0.07210661
6.26044157	-0.42909934	-0.43224316
-0.06725166	3.44700032	-0.06417919
-0.43209135	6.24981615	-0.40803825

EQ1

-0.53392556	2.00357520	1.34026952
1.48796931	-1.19842250	3.61231325
0.75195680	-2.99261561	5.65270790
2.35876145	0.90666596	1.21465275
5.07717682	-0.09307337	1.06656380
-0.20253853	4.18632132	-0.91686350
0.06059970	6.18754900	-2.96964373

EQ2

2.25277581	-0.03163547	-1.21516679
1.28573504	1.28574552	1.28576816
0.31867663	2.60313753	3.78667800
4.61642531	-1.89865571	-0.15990706
6.74815614	-3.59962472	0.70105030
-2.04500551	4.47007415	2.73131605
-4.17676341	6.17095871	1.87026135

EQ3

-0.62883404	-0.81933072	-0.90794727
1.08054916	-0.09151596	3.22290905
0.25674009	-0.21799892	5.89512710
2.06701606	0.06146732	0.02285300
4.82504311	0.84448590	0.85320808
1.10261292	3.27120593	-0.02380334

EQ4

3.16110715	1.73107487	-0.85821963
1.04974176	2.47025814	0.97737826
0.71491798	4.27895053	4.99172526
3.93581596	-1.35140399	-0.22144027
4.72949084	-4.03882186	0.21152829
-1.22577262	3.36406580	2.91012572
-3.36530108	2.54587651	0.98890237

EQ5

-2.05438291	0.69566427	0.33635955
1.63728344	0.10737227	3.09313857
1.12101501	-0.71969376	5.71454475
2.33816738	1.08401020	-0.04228530
4.59545290	-0.63155317	-0.28888045
-0.19962144	3.02226080	0.18011580
1.56208562	5.44193939	0.00700709

Acetonitrile

EQ0

0.04340934	0.04635128	0.04397486
-0.04787752	-0.04916052	3.23906820
-0.12330266	-0.13267544	6.06659589
3.23825236	-0.04764124	-0.04486490
6.06575996	-0.12596359	-0.12221744
-0.04796786	3.24115019	-0.05021595
-0.12827364	6.06793931	-0.13234065

EQ1

-0.55741836	1.97346773	1.37780321
1.48810206	-1.16553645	3.58063857
0.74803406	-2.93883282	5.60294111
2.35052928	0.94995658	1.17550502
5.04171334	-0.05726117	1.04621377
-0.20064818	4.13298645	-0.86593654
0.12968779	6.10521968	-2.91716513

EQ2

2.10337235	0.08217785	-1.30428399
1.28573103	1.28576789	1.28586420
0.46804792	2.48938368	3.87595411
4.44193588	-1.74585895	-0.15806326
6.53123992	-3.38122682	0.85332159
-1.87052652	4.31728039	2.72945849
-3.95980058	5.95247596	1.71774885

EQ3

-0.64928758	-0.75627151	-0.84145510
1.09126673	-0.10759171	3.20739232
0.27666944	-0.25485163	5.86155305
2.07837411	0.04554660	0.00534524
4.77324588	0.89667475	0.90611617
1.11079786	3.25603245	-0.03746534
0.31893356	5.92046105	-0.10148634

EQ4

3.19852654	1.92657731	-1.0141582
1.13166376	2.49856229	0.86390931
0.85073804	4.03120581	4.94269885
3.82790052	-1.1716082	-0.1854536
4.37860773	-3.8289672	0.51443006
-1.1539806	3.1784815	2.92055964
-3.233456	2.36574849	0.95801394

EQ5

-1.93477781	0.71703352	0.70297148
1.61166426	0.04819368	3.03987864
0.92194142	-0.86360235	5.57009758
2.40511921	1.14407407	-0.03943149
4.63982796	-0.54667615	-0.23866928
-0.19086207	3.06184144	0.22675819
1.54708702	5.43913580	-0.26160512

EQ6

1.7181179	-2.595928	0.92031638
-0.3330126	-0.5743203	1.65509928
-2.4701313	1.34865849	2.40949858
4.24283271	-0.7811231	0.26958055
6.53452754	0.78771792	-0.3253328
-0.9830742	4.14307269	2.14462818
0.29073996	6.67192235	1.92620985

EQ7

-2.4818205	1.81593841	2.74255481
1.58809412	-0.0222066	2.24881002
0.12403811	-1.3865918	4.13641605
3.51611427	1.79415773	-0.2386353
5.55556071	-0.0877898	0.54922188
-0.7600364	2.97481669	0.78948159
1.45804912	3.91167599	-1.2278488

EQ8

3.03306791	1.83971294	0.0185169
0.53268645	-0.092814	2.94675778
-2.1585251	0.46094105	3.51456777
3.6334322	-0.1929577	1.76551728
6.91501806	0.38753568	-0.1617658
-0.1680968	2.84364303	0.36158875
-2.7875863	3.75393925	0.55481653

EQ9

4.29482422	2.38308998	-0.406133
2.02058405	2.82937398	1.24508201
-0.6564249	5.43253383	3.79543509
2.99687956	-0.7794021	-0.4622344
1.57782905	-3.1461193	-0.2042424
-0.6336504	2.56057026	2.94188325
-0.6000409	-0.2800469	2.09020873

2. $\Delta\Delta G^{sol}$ of I_7^- of each structure in each phase.

Table S1. $\Delta\Delta G^{sol}$ of I_7^- of each structure in each phase (unit: kcal/mol).

	Gas phase	Acetonitrile
EQ0	0.00[a]	-0.69
EQ1	2.75	1.77
EQ2	0.72	0.00[b]
EQ3	7.32	6.19
EQ4	8.77	6.88
EQ5	8.72	6.85
EQ6	–	0.15
EQ7	–	0.65
EQ8	–	27.60
EQ9	–	5.60

a: Free energy is −2064.00527 hartree.
b: Free energy is −2064.03400 hartree.