Supplementary Information for

"Theoretical investigation for multi-spin excited states of anthracene-radical π-conjugated spin systems by computational chemistry"

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Table S1. Calculated exchange interaction (J_{DQ}) obtained using the broken-symmetry method, g value and D_{SS} value for Q state of **pOV0a** for various functionals and basis-sets by the DFT method.

Functional	Basis-set	J_{DQ} / cm^{-1}	g	D_{SS} / cm^{-1}
B3LYP	6-31G (d,p)	84.82	2.0028809	0.01402
	6-311G (2d, 2p)	66.97	2.0029693	0.01402
	Def2-SVP	68.53	2.0028976	0.01381
	Def2-TZVB	55.04	2.0029720	0.01395
CAM-B3LYP	6-31G (d,p)	88.62	2.0029098	0.01402
	6-311G (2d, 2p)	66.73	2.0030012	0.01401
	Def2-SVP	70.49	2.0029270	0.01382
	Def2-TZVB	54.09	2.0030030	0.01398
O3LYP	6-31G (d,p)	79.49	2.0028645	0.01423
	6-311G (2d, 2p)	68.76	2.0029455	0.01427
	Def2-SVP	64.28	2.0028827	0.01404
	Def2-TZVB	64.36	2.0029558	0.01417
B3PW91	6-31G (d,p)	87.78	2.0028722	0.01396
	6-311G (2d, 2p)	73.34	2.0029577	0.01400
	Def2-SVP	68.22	2.0028929	0.01395
	Def2-TZVB	67.42	2.0029623	0.01394

Table S2. Calculated exchange interaction (J_{DQ}) for Q state of **pOV0a** obtained by CASSCF method.

Method	Basis-set	J_{DQ} / cm^{-1}
CASSCF (3e, 3o)	6-31G (d,p)	53.5
CASSCF (3e, 3o)/ QD-NEVPT2	Def2-TZVB/RI-JK	7.87
CASSCF (13e, 13o)	6-31G (d,p)	32.3
CASSCF (13e, 13o) / NEVPT2	6-31G (d,p)	8.34
CASSCF (13e, 13o) / QD-NEVPT2	6-31G (d,p)	11.8

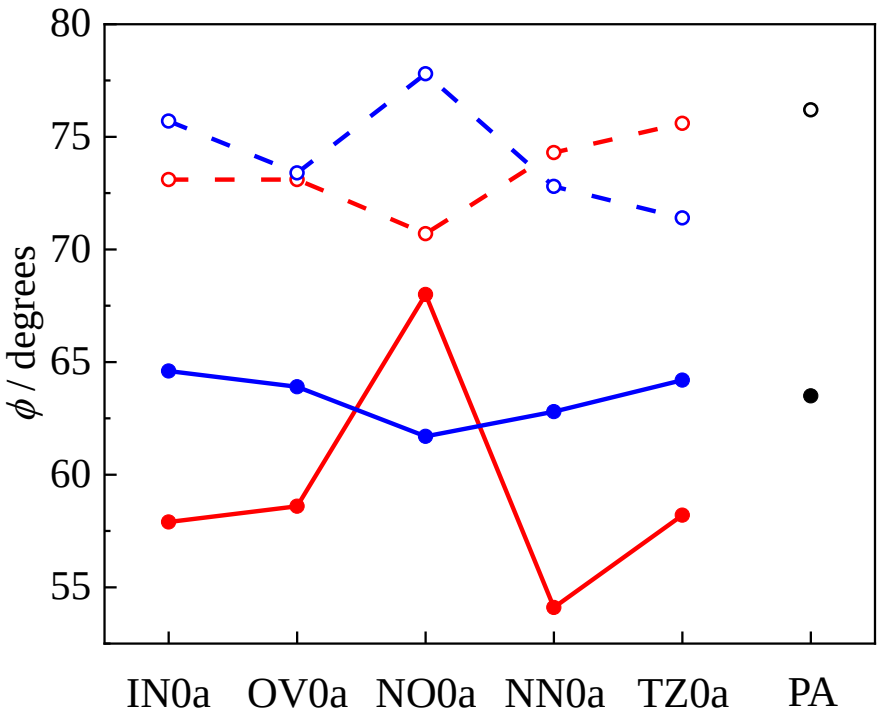

Fig. S1. Dihedral angles in Q state between the anthracene and phenyl moiety for each radical substituent; para (red) joint, meta (blue) joint and phenylanthracene (black). Open and closed circles correspond to the ground state and excited state, respectively.

Table S3. Results of the calculation for anthracene-radical linked π-conjugated spin systems

Sample	State	ϕ / º	Total Energy / Hartree	$<S^2>$	ΔE_{DQ} / cm^{-1}	J_{DQ} / cm^{-1}	$r_{An\text{-}R}$ / Å
***p*IN0a**	D	58.6	-1227.79977	1.778833	102.0797566	50.65374478	5.792
	Q		-1227.800235	3.794079			
	D_0	73.1	-1227.863991	0.769468			
***p*IN1a**	D	57.1	-1534.821701	1.789118	25.16585529	12.55439151	12.685
	Q		-1534.821816	3.793664			
	D_0	71.6	-1534.885511	0.770315			
***p*IN2a**	D	58.5	--	--	--	--	19.574
	Q		-1841.843517	3.792421			
	D_0	75.2	-1841.907264	0.770462			
***p*IN3a**	D	58.3	--	--	--	--	26.463
	Q		-2148.865286	3.792113			
	D_0	74.9	-2148.929013	0.770454			
***p*IN4a**	D	58.1	--	--	--	--	33.351
	Q		-2455.887053	3.792061			
	D_0	74.3	-2455.950745	0.770441			
***p*IN5a**	D	58.2	--	--	--	--	40.237
	Q		-2762.908813	3.791986			
	D_0	72	-2762.97245	0.77045			
***p*IN0b**	D	1.4	-1303.926554	1.777757	316.5743791	155.9487382	8.320
	Q		-1303.927996	3.807747			
	D_0	3.0	-1303.981464	0.770371			
***p*IN1b**	D	0.7	-1610.949499	1.796768	66.07258909	32.87165685	15.210
	Q		-1610.949800	3.806785			
	D_0	1.9	-1611.003214	0.770319			
***p*IN2b**	D	1.0	-1917.971458	1.801424	12.79642489	6.389095207	22.097
	Q		-1917.971517	3.804278			
	D_0	4.6	-1918.024982	0.770426			
***p*IN3b**	D	1.0	-2224.993262	1.80259	2.423414401	1.211272354	28.976
	Q		-2224.993273	3.803308			
	D_0	4.9	-2225.046749	0.770416			

***p*IN4b**	D	0.2	-2532.014989	1.802956	0.431302751	0.215633154	35.873
	Q		-2532.014991	3.803125			
	D_0	2.9	-2532.068428	0.770452			
***p*IN0a**	D	63.9	-1227.799026	1.792665	-26.71643238	-13.38817222	5.792
	Q		-1227.798904	3.78819			
	D_0	73.4	-1227.863386	0.769387			
***m*IN1a**	D	58.1	-1534.819377	1.7921	-7.621582493	-3.81405417	11.472
	Q		-1534.819343	3.790389			
	D_0	72.2	-1534.88438	0.769666			
***m*IN2a**	D	57.2	-1841.842311	1.791556	-1.62093627	-0.810665127	18.249
	Q		-1841.842303	3.79107			
	D_0	72.6	-1841.906063	0.769663			
***m*IN3a**	D	58.8	-2148.864048	1.790998	-0.270987483	-0.13550072	25.105
	Q		-2148.864047	3.790895			
	D_0	75.0	-2148.927944	0.769578			
***m*IN4a**	D	58.1	-2455.885923	1.791205	-0.079934818	-0.039968049	31.94
	Q		-2455.885923	3.791173			
	D_0	73.1	-2455.949700	0.769696			
***m*IN5a**	D	57.0	-2762.907685	1.791345	-0.015898716	-0.007949378	38.834
	Q		-2762.907685	3.79134			
	D_0	73.1	-2762.971468	0.769722			
***m*IN0b**	D	1.2	-1303.924159	1.804668	-88.95481336	-44.76033677	7.264
	Q		-1303.923754	3.792026			
	D_0	0.8	-1303.980224	0.769653			
***m*IN1b**	D	0.0	-1610.948417	1.803835	-20.60692885	-10.32515758	13.895
	Q		-1610.948323	3.799633			
	D_0	0.0	-1611.000879	0.770011			
***m*IN2b**	D	0.2	-1917.970361	1.8028	-4.148752507	-2.075571783	20.695
	Q		-1917.970342	3.801648			
	D_0	1.0	-1918.023858	0.769672			
***m*IN3b**	D	0.2	-2224.990995	1.802714	-0.806485671	-0.403300104	27.522
	Q		-2224.990991	3.80243			
	D_0	0.2	-2225.034546	0.770001			
***m*IN4b**	D	0.3	-2532.0128	1.802599	-0.138161542	-0.06908312	34.344

	Q		-2532.012799	3.802531			
	D_0	0.0	-2532.066289	0.770009			
***p*OV0a**	D	57.9	-1219.407667	1.791571	148.3943621	73.93077	5.801
	Q		-1219.408343	3.798778			
	D_0	73.1	-1219.472056	0.774374			
***p*OV1a**	D	57.3	-1526.429746	1.794654	33.57934167	16.78326	12.694
	Q		-1526.429899	3.795418			
	D_0	73.8	-1526.493680	0.775339			
***p*OV2a**	D	58.3	-1833.451640	1.796222	6.470587472	3.233224	19.585
	Q		-1833.451669	3.797502			
	D_0	74.3	-1833.515445	0.775406			
***p*OV3a**	D	58.2	-2140.473435	1.796717	1.233892814	0.616841	26.474
	Q		-2140.473441	3.797058			
	D_0	73.6	-2140.537236	0.775402			
***p*OV4a**	D	58.0	-2447.495205	1.796894	0.247238167	0.123614	33.360
	Q		-2447.495206	3.796974			
	D_0	73.6	-2447.558966	0.775399			
***p*OV5a**	D	58.0	-2754.516973	1.796894	0.039239927	0.01962	40.242
	Q		-2754.516973	3.796934			
	D_0	73.3	-2754.580718	0.775403			
***p*OV0b**	D	0.1	-1295.534266	1.793046	452.5772032	225.6419	8.399
	Q		-1295.536328	3.798778			
	D_0	2.3	-1295.589548	0.775663			
***p*OV1b**	D	1.0	-1602.557536	1.802684	90.04512808	44.81186	15.220
	Q		-1602.557946	3.812088			
	D_0	3.4	-1602.611317	0.775413			
***p*OV2b**	D	0.4	-1909.579571	1.806394	17.14164227	8.557706	22.111
	Q		-1909.579649	3.809459			
	D_0	1.0	-1909.633104	0.775399			
***p*OV3b**	D	0.1	-2216.601395	1.807566	3.21393339	1.60631	29.000
	Q		-2216.601409	3.808384			
	D_0	0.3	-2216.654886	0.775408			
***p*OV4b**	D	0.0	-2523.623180	1.807871	0.606305095	0.304813	35.831
	Q		-2523.623183	3.796974			

	D_0	0.8	-2523.676664	0.775404			
***m*OV0a**	D	64.6	-1219.407316	1.792757	-51.32328808	-25.66377413	5.015
	Q		-1219.407082	3.792591			
	D_0	75.7	-1219.471681	0.774205			
***m*OV1a**	D	57.7	-1526.428746	1.795924	-15.67742183	-7.844025242	11.529
	Q		-1526.428675	3.794569			
	D_0	71.9	-1526.492567	0.774211			
***m*OV2a**	D	57.3	-1833.450629	1.79606	-3.255894713	-1.628402495	18.376
	Q		-1833.450614	3.795501			
	D_0	71.3	-1833.51433	0.774207			
***m*OV3a**	D	57.8	-2140.47242	1.795817	-0.583207609	-0.291625677	25.261
	Q		-2140.472418	3.795667			
	D_0	71.7	-2140.53616	0.774202			
***m*OV4a**	D	57.5	-2447.493783	1.795822	-0.100473291	-0.050237751	31.602
	Q		-2447.493783	3.795778			
	D_0	70.9	-2447.55746	0.774196			
***m*OV5a**	D	57.6	-2754.515808	1.795782	-0.007710074	-0.003855056	38.543
	Q		-2754.515808	3.795772			
	D_0	73.4	-2754.579605	0.774189			
***m*OV0b**	D	0.5	-1295.533412	1.797127	-182.7566158	-91.44529155	7.335
	Q		-1295.532579	3.795662			
	D_0	2.2	-1295.587947	0.774705			
***m*OV1b**	D	2.1	-1602.556626	1.80687	-39.42844288	-19.74662565	14.080
	Q		-1602.556446	3.803588			
	D_0	4.0	-1602.609779	0.774651			
***m*OV2b**	D	1.3	-1909.578537	1.8072	-7.801290517	-3.903149129	20.665
	Q		-1909.578501	3.805917			
	D_0	11.1	-1909.631774	0.774209			
***m*OV3b**	D	1.1	-2216.600266	1.806912	-1.470791431	-0.735528846	27.432
	Q		-2216.600259	3.80655			
	D_0	3.4	-2216.653752	0.774191			
***m*OV4b**	D	1.7	-2523.621874	1.806803	-0.253043254	-0.126527194	34.200
	Q		-2523.621873	3.806715			
	D_0	5.6	-2523.675383	0.774185			

***p*NO0a**	D	68	-1057.016993	1.720346	-447.3831063	-217.2912397	5.801
	Q		-1057.014955	3.779256			
	D_0	70.7	-1057.079929	0.762029			
***p*NO1a**	D	61.9	-1364.038712	1.775148	-141.172028	-70.27410242	12.638
	Q		-1364.038069	3.784025			
	D_0	75.2	-1364.102308	0.76678			
***p*NO2a**	D	59.1	-1671.060409	1.787384	-33.77530611	-16.89207878	19.521
	Q		-1671.060255	3.78686			
	D_0	73.9	-1671.124138	0.767299			
***p*NO3a**	D	58.0	-1978.082157	1.788881	-6.865499094	-3.433855249	26.408
	Q		-1978.082126	3.788237			
	D_0	76.0	-1978.145879	0.767308			
***p*NO4a**	D	58.9	-2285.103761	1.788749	-1.142946855	-0.571530581	33.287
	Q		-2285.103756	3.788549			
	D_0	75.3	-2285.167654	0.767291			
***p*NO5a**	D	58.1	-2592.123377	1.78129	-0.128607662	-0.064305053	40.174
	Q		-2592.123377	3.781252			
	D_0	73.0	-2592.187103	0.75968			
***p*NO0b**	D	0.9	-1133.149261	1.347395	-2078.815416	-856.7809856	8.299
	Q		-1133.139789	3.773704			
	D_0	1.0	-1133.198258	0.770672			
***p*NO1b**	D	0.2	-1440.167596	1.747331	-462.0670742	-226.5348939	15.172
	Q		-1440.16549	3.787048			
	D_0	1.0	-1440.220038	0.767513			
***p*NO2b**	D	0.3	-1747.188566	1.794618	-94.24745872	-47.11006744	22.057
	Q		-1747.188136	3.795198			
	D_0	1.3	-1747.241826	0.767256			
***p*NO3b**	D	0.5	-2054.210172	1.799866	-17.94058908	-8.976371544	28.942
	Q		-2054.21009	3.798512			
	D_0	1.7	-2054.263613	0.767346			
***p*NO4b**	D	0.2	-2361.231878	1.79975	-3.277304388	-1.639077535	35.820
	Q		-2361.231864	3.799231			
	D_0	1.3	-2361.285399	0.767326			
***m*NO0a**	D	61.7	-1057.014833	1.776833	178.8051248	88.98845463	5.004

	Q		-1057.015648	3.78614			
	D_0	77.8	-1057.079897	0.761636			
***m*NO1a**	D	57.7	--	--	--	--	11.536
	Q		-1364.036734	3.786921			
	D_0	76.9	-1364.100548	0.762846			
***m*NO2a**	D	57.8	--	--	--	--	18.333
	Q		-1671.058503	3.785376			
	D_0	74	-1671.122273	0.762688			
***m*NO3a**	D	57.9	--	--	--	--	25.174
	Q		-1978.08028	3.784722			
	D_0	73.8	-1978.144045	0.762619			
***m*NO4a**	D	58.3	--	--	--	--	32.049
	Q		-2285.102075	3.784488			
	D_0	73.8	-2285.165763	0.762882			
***m*NO5a**	D	58.0	--	--	--	--	38.858
	Q		-2592.123815	3.784418			
	D_0	73.6	-2592.187546	0.76287			
***m*NO0b**	D	0.6	-1133.139942	1.773243	510.7526616	251.9724351	7.333
	Q		-1133.142269	3.800261			
	D_0	2.2	-1133.196211	0.762967			
***m*NO1b**	D	0.3	-1440.164206	1.78807	117.3219274	58.29310505	14.006
	Q		-1440.16474	3.800691			
	D_0	1.1	-1440.218165	0.762658			
***m*NO2b**	D	0.1	-1747.186394	1.793106	23.23673722	11.59411373	20.825
	Q		-1747.1865	3.79729			
	D_0	0.9	-1747.239953	0.762645			
***m*NO3b**	D	0	-2054.208241	1.794629	4.399974061	2.198741443	27.677
	Q		-2054.208261	3.795762			
	D_0	0.8	-2054.261729	0.762661			
***m*NO4b**	D	0	-2361.230028	1.79508	0.835074556	0.417479039	34.571
	Q		-2361.230032	3.795359			
	D_0	1.1	-2361.283499	0.762665			
***p*NN0a**	D	54.1	-1302.938853	1.826672	437.0494871	217.0771645	5.783
	Q		-1302.940844	3.840009			

	D_0	74.3	-1303.003879	0.814829			
***p*NN1a**	D	56.2	--	--	--	--	12.678
	Q		-1609.961874	3.843416			
	D_0	70.0	-1610.025397	0.818019			
***p*NN2a**	D	57.4	--	--	--	--	19.565
	Q		-1916.983637	3.842294			
	D_0	73.1	-1917.047332	0.819551			
***p*NN3a**	D	58.1	--	--	--	--	26.445
	Q		-2224.005412	3.841382			
	D_0	73.4	-2224.069189	0.819706			
***p*NN4a**	D	58.0	--	--	--	--	33.331
	Q		-2531.027133	3.840738			
	D_0	76.8	-2531.089148	0.815233			
***p*NN5a**	D	58.6	-2838.048885	1.840922	0.079315924	0.039657407	40.202
	Q		-2838.048885	3.84095			
	D_0	75.4	-2838.111366	0.815719			
***p*NN0b**	D	0.3	--	--	--	--	8.303
	Q		-1379.069728	3.850312			
	D_0	7.4	-1379.120945	0.816896			
***p*NN1b**	D	0.0	--	--	--	--	15.205
	Q		-1686.090205	3.858818			
	D_0	6.5	-1686.141844	0.814845			
***p*NN2b**	D	0.1	--	--	--	--	22.102
	Q		-1993.109919	3.850688			
	D_0	0.4	-1993.163329	0.815512			
***p*NN3b**	D	1.3	--	--	--	--	28.992
	Q		-2300.131778	3.848982			
	D_0	10.1	-2300.186503	0.818515			
***p*NN4b**	D	0.2	-2607.153395	1.847943	1.122700313	0.561249973	35.882
	Q		-2607.153401	3.8483			
	D_0	2.2	-2607.208244	0.819711			
***m*NN0a**	D	62.8	-1302.938506	1.823837	-60.95761282	-30.3935828	5.009
	Q		-1302.938228	3.829445			
	D_0	72.8	-1303.002737	0.81324			

***m*NN1a**	D	58.9	-1609.960162	1.836946	-15.89319387	-7.960691339	11.445
	Q		-1609.96009	3.833405			
	D_0	72.3	-1610.022232	0.811169			
***m*NN2a**	D	57.7	-1916.982001	1.83657	-3.411491227	-1.706618549	18.301
	Q		-1916.981985	3.835547			
	D_0	73.9	-1917.045866	0.814719			
***m*NN3a**	D	58.1	-2224.003782	1.835912	-0.661250714	-0.330667517	24.932
	Q		-2224.003779	3.835657			
	D_0	73.4	-2224.067625	0.814791			
***m*NN4a**	D	57.5	-2531.025446	1.834732	-0.116911955	-0.058457643	31.932
	Q		-2531.025446	3.834675			
	D_0	71.8	-2531.089361	0.81462			
***m*NN5a**	D	56.9	-2838.047295	1.836288	-0.033224051	-0.016612142	38.837
	Q		-2838.047295	3.836274			
	D_0	70.5	-2838.110984	0.814091			
***m*NN0b**	D	2.9	-1379.065335	1.855262	-192.1893421	-97.4224909	7.316
	Q		-1379.064459	3.828003			
	D_0	7.8	-1379.11993	0.814483			
***m*NN1b**	D	0.7	-1686.086564	1.84709	-41.41971178	-20.79754875	13.952
	Q		-1686.086375	3.838657			
	D_0	0.8	-1686.141673	0.814346			
***m*NN2b**	D	0.0	-1993.109938	1.847992	-8.962124562	-4.486636928	20.792
	Q		-1993.109897	3.845507			
	D_0	0.1	-1993.163436	0.814274			
***m*NN3b**	D	0.1	-2300.131726	1.847165	-1.707975493	-0.854244447	27.629
	Q		-2300.131718	3.846564			
	D_0	0.5	-2300.185218	0.8143			
***m*NN4b**	D	0.0	-2607.153496	1.847024	-0.320909192	-0.160465508	34.463
	Q		-2607.153494	3.846888			
	D_0	0.5	-2607.206988	0.814303			
***p*TZ0a**	D	58.2	-1713.174126	1.786161	163.3562924	81.35974484	5.791
	Q		-1713.17487	3.793988			
	D_0	75.6	-1713.238597	0.769621			
***p*TZ1a**	D	57.4	-2020.196136	1.789929	34.20102544	17.06572424	12.683

	Q		-2020.196292	3.794006			
	D_0	74.9	-2020.260019	0.770494			
***p*TZ2a**	D	57.2	-2327.217943	1.79153	6.699664084	3.347674466	19.573
	Q		-2327.217973	3.792819			
	D_0	74.6	-2327.28174	0.770541			
***p*TZ3a**	D	57.5	-2634.239725	1.792003	1.263100492	0.631450793	26.464
	Q		-2634.239731	3.792318			
	D_0	75.8	-2634.303481	0.770563			
***p*TZ4a**	D	58	-2941.261504	1.792053	0.230871963	0.115431595	33.351
	Q		-2941.261505	3.792129			
	D_0	73.3	-2941.325169	0.770564			
***p*TZ5a**	D	58.2	-3248.283271	1.792068	0.051477777	0.025738657	40.241
	Q		-3248.283272	3.792086			
	D_0	73.2	-3248.347003	0.770543			
***p*TZ0b**	D	0.2	-1789.300639	1.788762	428.6143671	212.4126749	8.319
	Q		-1789.302592	3.8066			
	D_0	0.3	-1789.3559	0.770814			
***p*TZ1b**	D	0.7	-2096.323875	1.798066	86.76361195	43.18638757	15.209
	Q		-2096.32427	3.807116			
	D_0	0.6	-2096.377649	0.770579			
***p*TZ2b**	D	0.3	-2403.345888	1.801624	16.54235804	8.259025863	22.098
	Q		-2403.345963	3.804567			
	D_0	0.8	-2403.399418	0.770559			
***p*TZ3b**	D	0.2	-2710.367703	1.802715	3.095752907	1.54726451	28.987
	Q		-2710.367717	3.803506			
	D_0	0.9	-2710.42119	0.770549			
***p*TZ4b**	D	0.3	-3017.389483	1.803033	0.572813266	0.286381432	35.873
	Q		-3017.389485	3.803209			
	D_0	0.8	-3017.442965	0.770553			
***m*TZ0a**	D	64.2	-1713.173821	1.767564	-69.09834935	-34.20024666	5.011
	Q		-1713.173506	3.787969			
	D_0	71.4	-1713.238022	0.769481			
***m*TZ1a**	D	59.5	-2020.195161	1.788271	-15.88485607	-7.936499469	11.516
	Q		-2020.195088	3.789765			

	D_0	74.9	-2020.259039	0.769462			
***m*TZ2a**	D	58	-2327.216934	1.790859	-3.148837153	-1.574553988	18.257
	Q		-2327.21692	3.790687			
	D_0	74.6	-2327.280708	0.76947			
***m*TZ3a**	D	58.1	-2634.238706	1.790973	-0.59270001	-0.296363489	25.029
	Q		-2634.238703	3.790882			
	D_0	75.8	-2634.302395	0.76944			
***m*TZ4a**	D	58.1	-2941.260424	1.790967	-0.116997488	-0.058499534	31.734
	Q		-2941.260423	3.79094			
	D_0	73.3	-2941.324155	0.769444			
***m*TZ5a**	D	58.2	-3248.28226	1.79095	-0.027570469	-0.013785283	38.732
	Q		-3248.28226	3.790943			
	D_0	73.2	-3248.34593	0.769447			
***m*TZ0b**	D	1.8	-1789.30028	1.773037	-191.318186	-94.80180034	7.295
	Q		-1789.299409	3.791123			
	D_0	3.8	-1789.354768	0.769485			
***m*TZ1b**	D	1.9	-2096.322971	1.799955	-37.84949648	-18.93355234	13.998
	Q		-2096.322799	3.799025			
	D_0	9.6	-2096.376549	0.769428			
***m*TZ2b**	D	0.8	-2403.344858	1.802189	-7.345430774	-3.674431347	20.905
	Q		-2403.344824	3.801255			
	D_0	3.6	-2403.398319	0.76945			
***m*TZ3b**	D	0.3	-2710.366661	1.802125	-1.349494423	-0.674851138	27.551
	Q		-2710.366655	3.801817			
	D_0	2.0	-2710.420138	0.769437			
***m*TZ4b**	D	1.2	-3017.38819	1.802045	-0.244262067	-0.122135858	34.064
	Q		-3017.388189	3.801966			
	D_0	13	-3017.441505	0.769448			

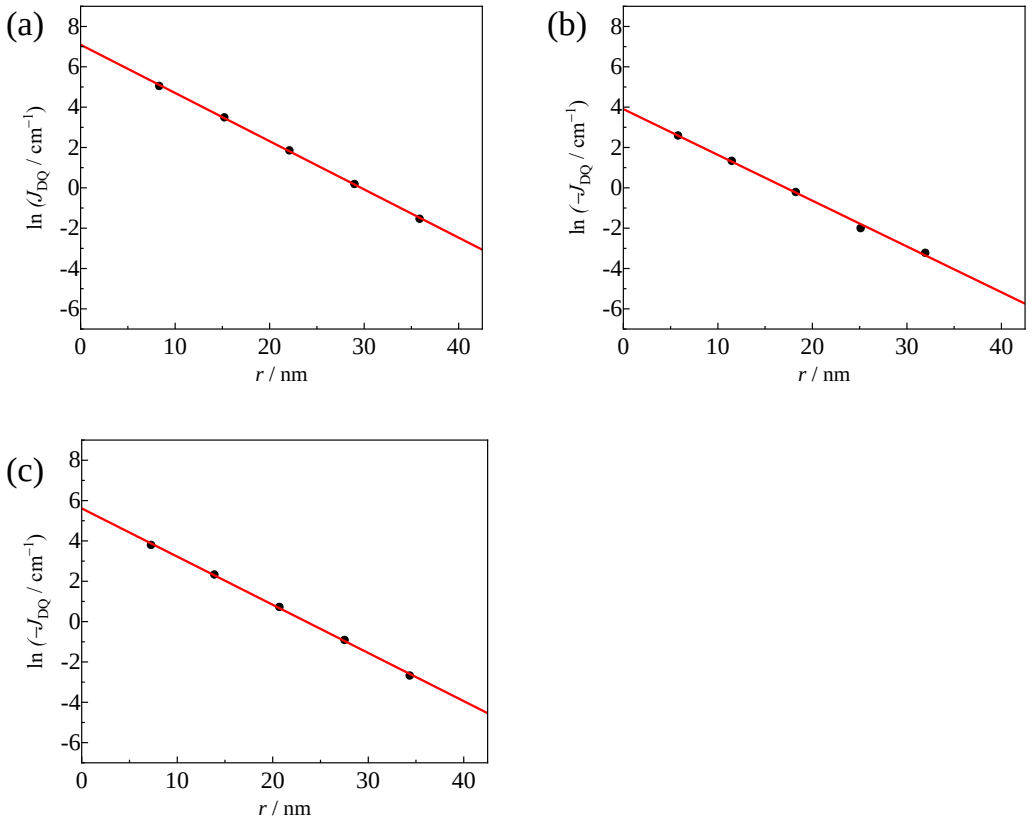

Fig. S2. Linker length dependence of J_{DQ}; (a) ***p*INN*n*b**, (b) ***m*INN*n*a** and (c) ***m*INN*n*b** series. The red lines are least-square fit using Eqn. 3.

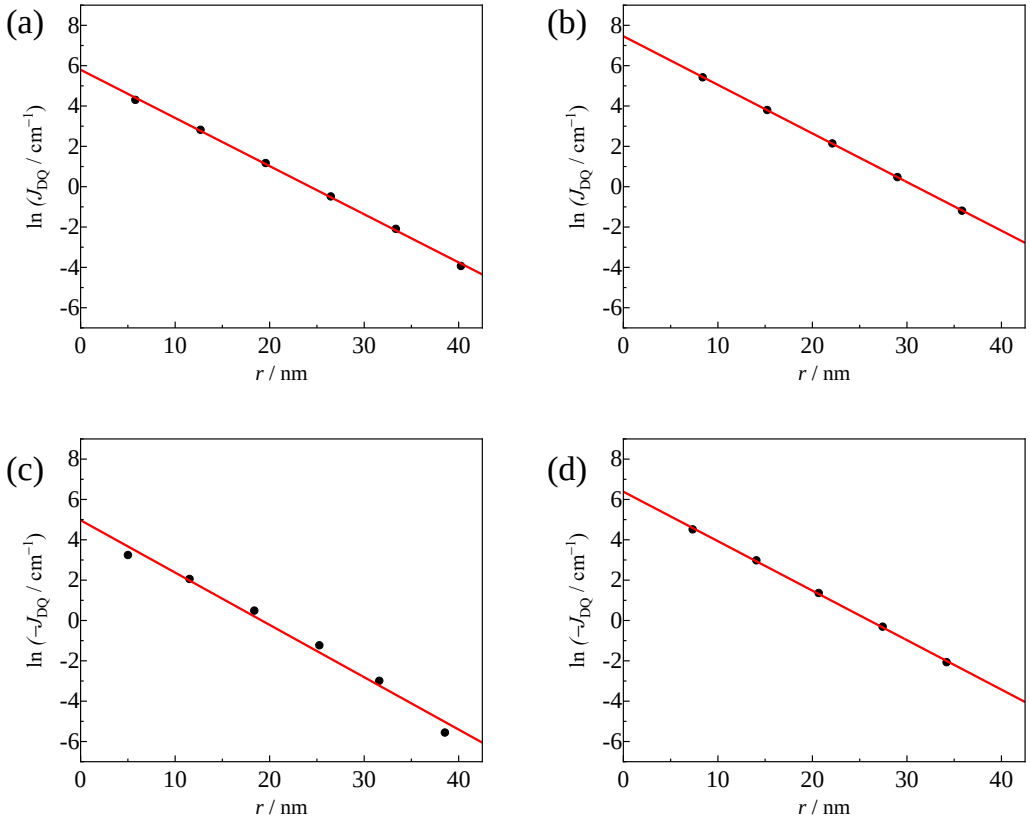

Fig. S3. Linker length dependence of J_{DQ}; (a) ***p*OV*n*a**, (b) ***p*OV*n*b**, (c) ***m*OV*n*a**, a***n***d (d) ***m*OV*n*b** series. The red lines are least-square fit using Eqn. 3.

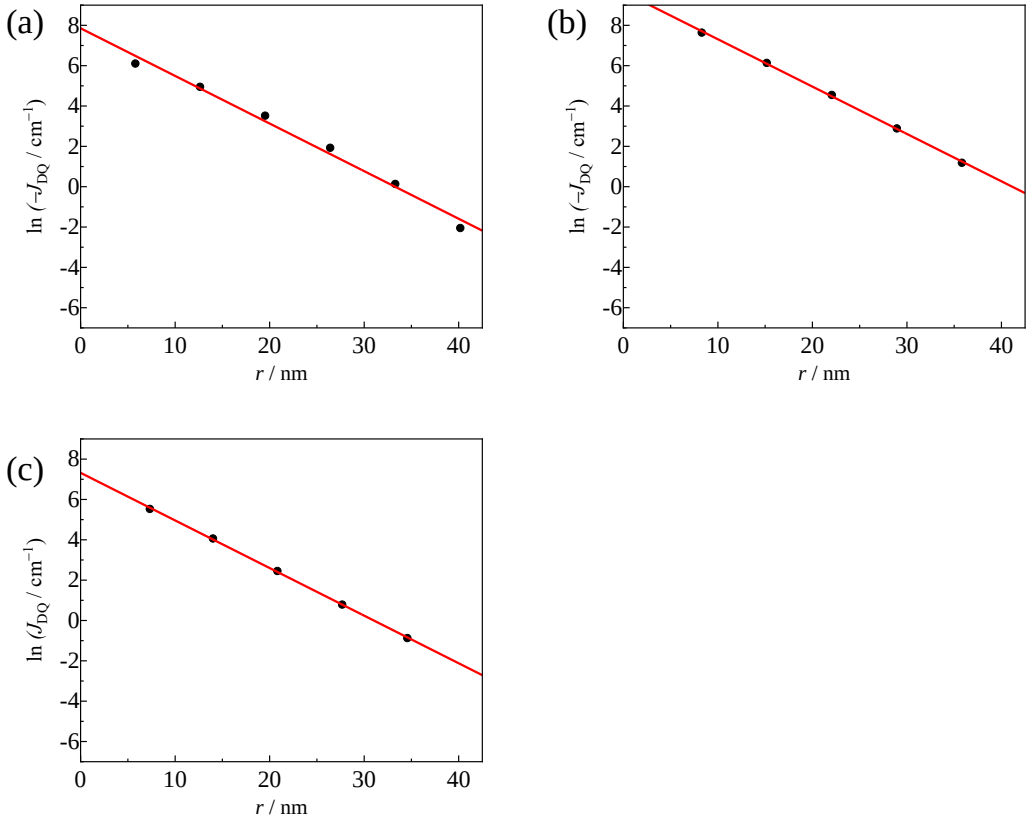

Fig. S4. Linker length dependence of J_{DQ}; (a) ***p*NO*n*a**, (b) ***p*NO*n*b**, and (c) ***m*NO*n*b** series. The red lines are least-square fit using Eqn. 3.

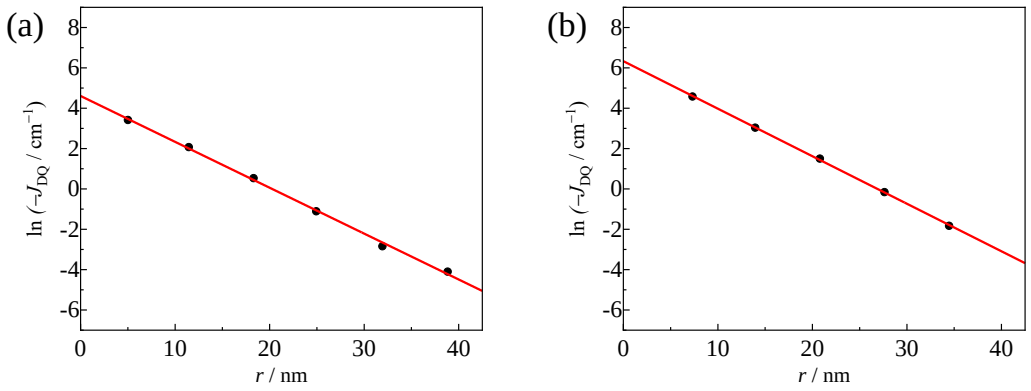

Fig. S5. Linker length dependence of J_{DQ}; (a) ***m*NN*n*a** and (d) ***m*NN*n*b** series. The red lines are least-square fit using Eqn. 3.

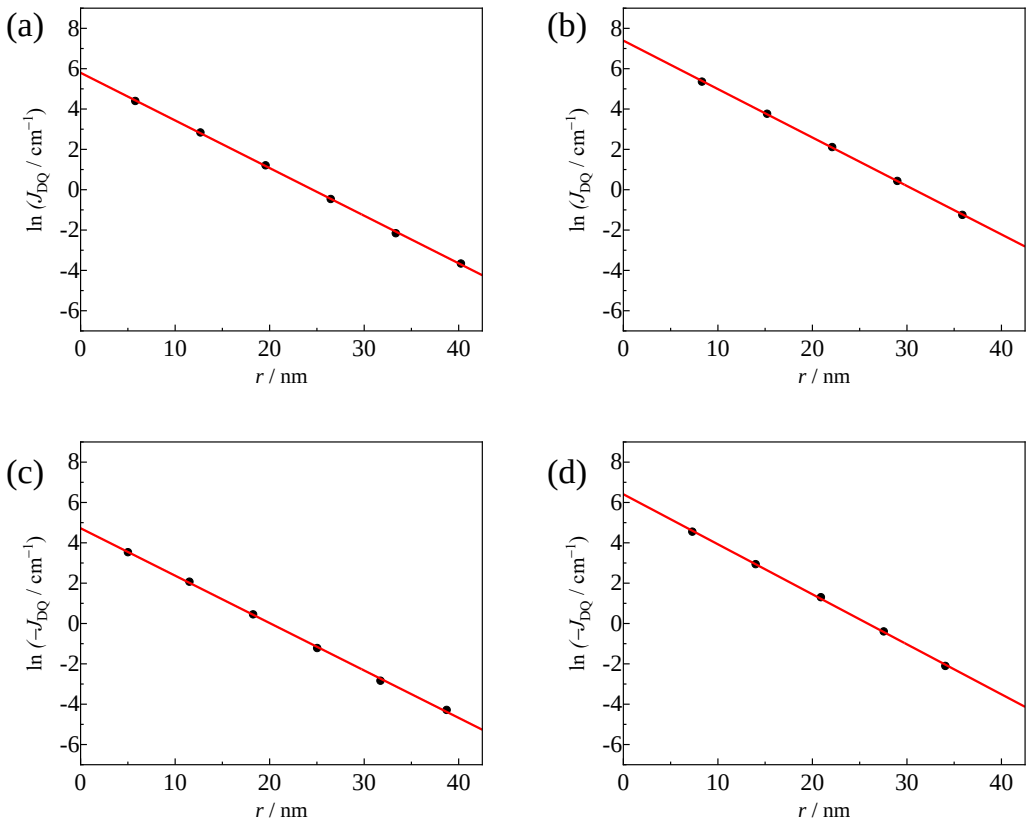

Fig. S6. Linker length dependence of J_{DQ}; (a) ***p*TZ*n*a**, (b) ***p*TZ*n*b**, (c) ***m*TZ*n*a** and (d) ***m*TZ*n*b** series. The red lines are least-square fit using Eqn. 3.

Table S4. Calculated decay constant (β) and J_0^{Ex} values of Q states for anthracene-radical linked π-conjugated spin systems

	β /	J_0^{Ex} / cm^{-1}
***p*INN*n*a**	--	--
***p*INN*n*b**	−0.239	1205
***m*INN*n*a**	−0.227	−50
***m*INN*n*b**	−0.239	−274
***p*OV*n*a**	−0.239	329
***p*OV*n*b**	−0.241	1737
***m*OV*n*a**	−0.259	−144
***m*OV*n*b**	−0.245	−593
***p*NO*n*a**	−0.236	−2574
***p*NO*n*b**	−0.235	−15634
***m*NO*n*a**	--	--
***m*NO*n*b**	−0.236	1512
***p*NN*n*a**	--	--
***p*NN*n*b**	--	--
***m*NN*n*a**	−0.227	−100
***m*NN*n*b**	−0.236	−562
***p*TZ*n*a**	−0.236	329
***p*TZ*n*b**	−0.240	1623
***m*TZ*n*a**	−0.235	−113
***m*TZ*n*b**	−0.248	−607

Table. S5 Experimental and calculated *g* values for Q states of anthracene-radical linked π-conjugated spin systems

.

	Experiment	Calculation by eq.3
***p*IN0a**	2.0043 (S= 3/2) [1]	2.00413
***p*OV0a**	2.0035 (S= 3/2) [2]	2.00303
***p*NO0a**	2.0048 (S= 3/2) [3]	2.00387
***p*NN0a**		2.00402
***p*TZ0a**		2.00526

Table. S6 Referenced *g* values used in the calculation of Eqn 3.

	Experiment
phenyl-*p*OV	2.0036 (S= 1/2) [4]
phenyl-*p*IN	2.0068 (S= 1/2) [5]
phenyl-*p*NO	2.0060 (S= 1/2) [6]
phenyl-*p*NN	2.00645 (S= 1/2) [7]
phenyl-*p*TZ	2.01019 (S= 1/2) [8]
Anthracene	2.0028 (S = 1) [9]

Table. S7 Details of the calculated *g* values of Q states by UB3LYP/6-31G (d,p).

Sample		g_{xx}	g_{yy}	g_{zz}	g_{iso}
***p*IN0a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002005	-0.0002005	-0.0002005	
	Δg_{DSO}	0.0000627	0.0001053	0.0000859	
	Δg_{PSO}	0.0001926	0.001451	0.0023748	
	g_{total}	2.002374	2.0036751	2.0045794	2.0035429
***p*IN1a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002002	-0.0002002	-0.0002002	
	Δg_{DSO}	0.0000671	0.0001055	0.0000809	
	Δg_{PSO}	0.0002451	0.0014419	0.0023908	
	g_{total}	2.0024312	2.0036664	2.0045908	2.0035628
***p*IN2a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002001	-0.0002001	-0.0002001	
	Δg_{DSO}	0.0000716	0.0001046	0.0000771	
	Δg_{PSO}	0.000282	0.0014357	0.0024914	
	g_{total}	2.0024727	2.0036595	2.0046876	2.0036066
***p*IN3a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002001	-0.0002001	-0.0002001	
	Δg_{DSO}	0.0000715	0.0001046	0.0000773	
	Δg_{PSO}	0.0002608	0.001434	0.0024464	
	g_{total}	2.0024514	2.0036577	2.0046428	2.003584
***p*IN4a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002001	-0.0002001	-0.0002001	
	Δg_{DSO}	0.0000716	0.0001044	0.0000774	
	Δg_{PSO}	0.0002406	0.0014322	0.0023989	
	g_{total}	2.0024313	2.0036558	2.0045954	2.0035608
***p*IN5a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002001	-0.0002001	-0.0002001	
	Δg_{DSO}	0.0000594	0.0001056	0.0000884	
	Δg_{PSO}	0.0001188	0.0014374	0.0024462	
	g_{total}	2.0022974	2.0036621	2.0046538	2.0035377
***p*IN0b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002006	-0.0002006	-0.0002006	

	$\Delta \boldsymbol{g}_{DSO}$	0.00004	0.0001069	0.0001074	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0000247	0.0015414	0.0025922	
	g_{total}	2.002134	2.003767	2.0048182	2.0035731
***p*IN1b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001998	-0.0001998	-0.0001998	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000402	0.0001066	0.0001066	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0000211	0.0015099	0.0026025	
	g_{total}	2.0021385	2.0037359	2.0048286	2.0035677
***p*IN2b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001997	-0.0001997	-0.0001997	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000402	0.0001066	0.0001064	
	$\Delta \boldsymbol{g}_{PSO}$	0.000062	0.0015041	0.0026424	
	g_{total}	2.0022219	2.0037303	2.0048684	2.0036069
***p*IN3b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001996	-0.0001996	-0.0001996	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000402	0.0001065	0.0001065	
	$\Delta \boldsymbol{g}_{PSO}$	0.0000115	0.0015019	0.0026421	
	g_{total}	2.0021713	2.0037281	2.0048683	2.0035892
***p*IN4b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001996	-0.0001996	-0.0001996	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000408	0.0001063	0.0001061	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0000488	0.0014981	0.0026317	
	g_{total}	2.0021117	2.003724	2.0048574	2.0035644
***p*OV0a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001852	-0.0001852	-0.0001852	
	$\Delta \boldsymbol{g}_{DSO}$	0.000056	0.0000822	0.0001003	
	$\Delta \boldsymbol{g}_{PSO}$	0.0001551	0.0008677	0.0009794	
	g_{total}	2.0023452	2.0030839	2.0032138	2.0028809
***p*OV1a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001848	-0.0001848	-0.0001848	
	$\Delta \boldsymbol{g}_{DSO}$	0.00005	0.0000879	0.0001001	
	$\Delta \boldsymbol{g}_{PSO}$	0.0000822	0.0009182	0.0009692	
	g_{total}	2.0022667	2.0031406	2.0032038	2.0028704
***p*OV2a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001847	-0.0001847	-0.0001847	

	$\Delta \boldsymbol{g}_{DSO}$	0.0000647	0.0000732	0.0001	
	$\Delta \boldsymbol{g}_{PSO}$	0.0001928	0.0007852	0.000967	
	g_{total}	2.0023921	2.002993	2.0032016	2.0028622
***p*OV3a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001847	-0.0001847	-0.0001847	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000653	0.0000725	0.0001	
	$\Delta \boldsymbol{g}_{PSO}$	0.0001808	0.0007775	0.0009665	
	g_{total}	2.0023807	2.0029846	2.0032011	2.0028555
***p*OV4a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001847	-0.0001847	-0.0001847	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000653	0.0000725	0.0001	
	$\Delta \boldsymbol{g}_{PSO}$	0.0001639	0.0007742	0.0009662	
	g_{total}	2.0023638	2.0029814	2.0032009	2.0028487
***p*OV5a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001847	-0.0001847	-0.0001847	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000652	0.0000726	0.0001	
	$\Delta \boldsymbol{g}_{PSO}$	0.000146	0.0007715	0.0009663	
	g_{total}	2.0023458	2.0029787	2.0032009	2.0028418
***p*OV0b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001858	-0.0001858	-0.0001858	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000359	0.0001016	0.0001019	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0000736	0.0010644	0.0010918	
	g_{total}	2.0020958	2.0032995	2.0033271	2.0029075
***p*OV1b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001845	-0.0001845	-0.0001845	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000362	0.0001011	0.0001007	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0000333	0.0010366	0.0010639	
	g_{total}	2.0021377	2.0032724	2.0032994	2.0029032
***p*OV2b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001842	-0.0001842	-0.0001842	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000364	0.0001009	0.0001004	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0000601	0.0010301	0.0010561	
	g_{total}	2.0021114	2.0032661	2.0032915	2.0028897
***p*OV3b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001842	-0.0001842	-0.0001842	

	Δg_{DSO}	0.0000363	0.0001009	0.0001004	
	Δg_{PSO}	-0.0000889	0.0010288	0.0010539	
	g_{total}	2.0020825	2.0032648	2.0032894	2.0028789
***p*OV4b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001842	-0.0001842	-0.0001842	
	Δg_{DSO}	0.0000364	0.0001009	0.0001003	
	Δg_{PSO}	-0.0001242	0.0010282	0.0010499	
	g_{total}	2.0020473	2.0032642	2.0032853	2.0028656
***m*NO0a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001942	-0.0001942	-0.0001942	
	Δg_{DSO}	0.0000617	0.0000811	0.0001043	
	Δg_{PSO}	0.0001778	0.0010545	0.0024926	
	g_{total}	2.0023645	2.0032607	2.004722	2.0034491
***m*NO1a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001944	-0.0001944	-0.0001944	
	Δg_{DSO}	0.000061	0.0000823	0.0001045	
	Δg_{PSO}	0.0002933	0.0012343	0.0025335	
	g_{total}	2.0024791	2.0034414	2.0047629	2.0035611
***m*NO2a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001945	-0.0001945	-0.0001945	
	Δg_{DSO}	0.0000595	0.0000838	0.0001045	
	Δg_{PSO}	0.0002541	0.0012064	0.0025349	
	g_{total}	2.0024384	2.003415	2.0047642	2.0035392
***m*NO3a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001945	-0.0001945	-0.0001945	
	Δg_{DSO}	0.0000576	0.0000856	0.0001045	
	Δg_{PSO}	0.0002111	0.0011852	0.0025357	
	g_{total}	2.0023936	2.0033956	2.004765	2.003518
***m*NO4a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001945	-0.0001945	-0.0001945	
	Δg_{DSO}	0.0000636	0.0000799	0.0001042	
	Δg_{PSO}	0.0002131	0.001112	0.0025384	
	g_{total}	2.0024015	2.0033168	2.0047674	2.0034952
***m*NO5a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001945	-0.0001945	-0.0001945	

	Δg_{DSO}	0.0000713	0.000072	0.0001046	
	Δg_{PSO}	0.000247	0.0010151	0.0025405	
	g_{total}	2.002443	2.0032118	2.0047699	2.0034749
***m*NO0b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001934	-0.0001934	-0.0001934	
	Δg_{DSO}	0.0000391	0.0001039	0.0001045	
	Δg_{PSO}	0.0001734	0.0013193	0.0025685	
	g_{total}	2.0023384	2.0035491	2.0047988	2.0035621
***m*NO1b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.000194	-0.000194	-0.000194	
	Δg_{DSO}	0.0000395	0.0001036	0.0001046	
	Δg_{PSO}	0.0001196	0.0013213	0.0025914	
	g_{total}	2.0022844	2.0035502	2.0048213	2.003552
***m*NO2b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001941	-0.0001941	-0.0001941	
	Δg_{DSO}	0.0000396	0.0001036	0.0001046	
	Δg_{PSO}	0.0000711	0.0013209	0.0025928	
	g_{total}	2.0022359	2.0035496	2.0048225	2.003536
***m*NO3b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001942	-0.0001942	-0.0001942	
	Δg_{DSO}	0.0000398	0.0001036	0.0001044	
	Δg_{PSO}	0.0000247	0.0013215	0.0025926	
	g_{total}	2.0021896	2.0035503	2.0048221	2.0035206
***m*NO4b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001941	-0.0001941	-0.0001941	
	Δg_{DSO}	0.00004	0.0001036	0.0001041	
	Δg_{PSO}	-0.0000215	0.0013214	0.0025865	
	g_{total}	2.0021436	2.0035501	2.0048158	2.0035032
***p*NN0a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002169	-0.0002169	-0.0002169	
	Δg_{DSO}	0.0000593	0.0001118	0.0000989	
	Δg_{PSO}	0.0001098	0.001766	0.0032592	
	g_{total}	2.0022714	2.0039802	2.0054605	2.003904
***p*NN1a**	g_e	2.0023193	2.0023193	2.0023193	

	Δg_{RMC}	-0.0002156	-0.0002156	-0.0002156	
	Δg_{DSO}	0.0000583	0.000111	0.0000993	
	Δg_{PSO}	0.0001648	0.0017409	0.0033762	
	g_{total}	2.0023268	2.0039556	2.0055791	2.0039538
***p*NN2a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002156	-0.0002156	-0.0002156	
	Δg_{DSO}	0.0000709	0.0001107	0.0000869	
	Δg_{PSO}	0.0001804	0.0017345	0.0032939	
	g_{total}	2.002355	2.0039489	2.0054845	2.0039295
***p*NN3a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002155	-0.0002155	-0.0002155	
	Δg_{DSO}	0.0000732	0.0001104	0.0000848	
	Δg_{PSO}	0.0001619	0.0017323	0.0032444	
	g_{total}	2.0023389	2.0039464	2.0054329	2.0039061
***p*NN4a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002155	-0.0002155	-0.0002155	
	Δg_{DSO}	0.0000553	0.0001109	0.000102	
	Δg_{PSO}	0.0000029	0.0017339	0.0033276	
	g_{total}	2.002162	2.0039486	2.0055334	2.0038814
***p*NN5a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002155	-0.0002155	-0.0002155	
	Δg_{DSO}	0.0000826	0.00011	0.0000758	
	Δg_{PSO}	0.0001723	0.0017309	0.0030977	
	g_{total}	2.0023586	2.0039447	2.0052773	2.0038602
***p*NN0b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002185	-0.0002185	-0.0002185	
	Δg_{DSO}	0.0000441	0.0001133	0.0001144	
	Δg_{PSO}	0.0000522	0.0018757	0.0035661	
	g_{total}	2.0021971	2.0040898	2.0057812	2.0040227
***p*NN1b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002157	-0.0002157	-0.0002157	
	Δg_{DSO}	0.0000435	0.0001122	0.0001132	
	Δg_{PSO}	0.0000133	0.0018126	0.0034453	
	g_{total}	2.0021604	2.0040284	2.005662	2.0039503
***p*NN2b**	g_e	2.0023193	2.0023193	2.0023193	

	Δg_{RMC}	-0.0002152	-0.0002152	-0.0002152	
	Δg_{DSO}	0.0000433	0.0001127	0.0001133	
	Δg_{PSO}	-0.0000319	0.0018045	0.0033862	
	g_{total}	2.0021154	2.0040212	2.0056036	2.0039134
***p*NN3b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002151	-0.0002151	-0.0002151	
	Δg_{DSO}	0.0000435	0.0001126	0.000113	
	Δg_{PSO}	-0.0000827	0.0018021	0.0033828	
	g_{total}	2.002065	2.0040188	2.0055999	2.0038946
***p*NN4b**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0002151	-0.0002151	-0.0002151	
	Δg_{DSO}	0.0000433	0.0001126	0.0001132	
	Δg_{PSO}	-0.0001371	0.0018012	0.0033818	
	g_{total}	2.0020103	2.0040179	2.0055992	2.0038758
***p*TZ0a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001881	-0.0001881	-0.0001881	
	Δg_{DSO}	0.0000703	0.0000986	0.000122	
	Δg_{PSO}	-0.0000027	0.0017286	0.0063989	
	g_{total}	2.0021988	2.0039584	2.0086521	2.0049364
***p*TZ1a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001878	-0.0001878	-0.0001878	
	Δg_{DSO}	0.0000727	0.0000959	0.0001217	
	Δg_{PSO}	-0.000126	0.0018511	0.0064861	
	g_{total}	2.0020783	2.0040785	2.0087393	2.0049654
***p*TZ2a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001877	-0.0001877	-0.0001877	
	Δg_{DSO}	0.0000663	0.0001024	0.0001216	
	Δg_{PSO}	-0.0001801	0.0018413	0.0065073	
	g_{total}	2.0020178	2.0040753	2.0087605	2.0049512
***p*TZ3a**	g_e	2.0023193	2.0023193	2.0023193	
	Δg_{RMC}	-0.0001877	-0.0001877	-0.0001877	
	Δg_{DSO}	0.0000625	0.0001061	0.0001217	
	Δg_{PSO}	-0.0002406	0.0018372	0.006512	
	g_{total}	2.0019535	2.0040749	2.0087652	2.0049312
***p*TZ4a**	g_e	2.0023193	2.0023193	2.0023193	

	$\Delta \boldsymbol{g}_{RMC}$	-0.0001877	-0.0001877	-0.0001877	
	$\Delta \boldsymbol{g}_{DSO}$	0.000074	0.0000947	0.0001217	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0001994	0.0017349	0.0065094	
	g_{total}	2.0020061	2.0039612	2.0087627	2.00491
***p*TZ5a**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001877	-0.0001877	-0.0001877	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000736	0.0000951	0.0001216	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0002278	0.0016921	0.0065104	
	g_{total}	2.0019773	2.0039188	2.0087636	2.0048866
***p*TZ0b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001882	-0.0001882	-0.0001882	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000452	0.000123	0.0001231	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0002701	0.0019899	0.0062752	
	g_{total}	2.0019062	2.004244	2.0085294	2.0048932
***p*TZ1b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001874	-0.0001874	-0.0001874	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000452	0.0001224	0.0001227	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0003253	0.0019583	0.006514	
	g_{total}	2.0018518	2.0042126	2.0087686	2.0049444
***p*TZ2b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001872	-0.0001872	-0.0001872	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000452	0.0001224	0.0001226	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0003749	0.0019528	0.006563	
	g_{total}	2.0018024	2.0042072	2.0088176	2.0049424
***p*TZ3b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001872	-0.0001872	-0.0001872	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000453	0.0001224	0.0001225	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0004258	0.0019525	0.0065718	
	g_{total}	2.0017516	2.004207	2.0088264	2.0049283
***p*TZ4b**	g_e	2.0023193	2.0023193	2.0023193	
	$\Delta \boldsymbol{g}_{RMC}$	-0.0001872	-0.0001872	-0.0001872	
	$\Delta \boldsymbol{g}_{DSO}$	0.0000453	0.0001224	0.0001225	
	$\Delta \boldsymbol{g}_{PSO}$	-0.0004773	0.0019549	0.0065719	
	g_{total}	2.0017001	2.0042094	2.0088265	2.004912

Table. S8 Calculated zero-field splitting parameters for the T_1 state of the molecules without stable radical moiety by UB3LYP/6-31G (d, p).

	D_{SS} / cm^{-1}	E_{SS} / cm^{-1}
An-ph	0.03818	0.00047
An-ph$(CCph)_1$	0.03728	0.00057
An-ph$(CCph)_2$	0.03711	0.00059
An-ph$(CCph)_3$	0.03707	0.00060
An-ph$(CCph)_4$	0.03706	0.00060
An-ph$(CCph)_5$	0.03704	0.00061
An-$(CCph)_1$	0.03142	0.00353
An-$(CCph)_2$	0.02960	0.00415
An-$(CCph)_3$	0.02931	0.00424
An-$(CCph)_4$	0.02926	0.00426
An-$(CCph)_5$	0.02925	0.00426

Table. S9. Calculated zero-field splitting parameters for the Q state of anthracene-radical linked π-conjugated spin systems by UB3LYP/6-31G (d, p).

	D_{SS} / cm^{-1}	E_{SS} / cm^{-1}
***p*IN0a**	0.01402	0.00201
***p*IN1a**	0.01259	0.00054
***p*IN2a**	0.01245	0.0003
***p*IN3a**	0.01239	0.00024
***p*IN4a**	0.01236	0.00022
***p*IN5a**	0.01236	0.00021
***p*IN0b**	0.01302	0.00259
***p*IN1b**	0.01033	0.00173
***p*IN2b**	0.00988	0.00152
***p*IN3b**	0.00979	0.00146
***p*IN4b**	0.00977	0.00144
***p*OV0a**	0.01402	0.00206
***p*OV1a**	0.01263	0.00053
***p*OV2a**	0.01244	0.0003
***p*OV3a**	0.01239	0.00024
***p*OV4a**	0.01236	0.00022
***p*OV5a**	0.01236	0.00021
***p*OV0b**	0.0133	0.0028
***p*OV1b**	0.01035	0.00177
***p*OV2b**	0.00988	0.00152
***p*OV3b**	0.00979	0.00146
***p*OV4b**	0.00977	0.00144
***m*NO0a**	0.01532	0.00318
***m*NO1a**	0.01274	0.00066
***m*NO2a**	0.01245	0.00033
***m*NO3a**	0.01238	0.00025
***m*NO4a**	0.01238	0.00022
***m*NO5a**	0.01236	0.00021

***m*NO0b**	0.01358	0.00176
***m*NO1b**	0.01253	0.00051
***m*NO2b**	0.0124	0.0003
***m*NO3b**	0.01236	0.00022
***m*NO4b**	0.01238	0.00021
***p*NN0a**	0.01287	0.00165
***p*NN1a**	0.01025	0.00163
***p*NN2a**	0.00986	0.0015
***p*NN3a**	0.00979	0.00146
***p*NN4a**	0.00977	0.00144
***p*NN5a**	0.01383	0.00185
***p*NN0b**	0.01258	0.00051
***p*NN1b**	0.01239	0.0003
***p*NN2b**	0.01235	0.00024
***p*NN3b**	0.01236	0.00022
***p*NN4b**	0.01236	0.00021
***p*TZ0a**	0.01280	0.00265
***p*TZ1a**	0.01027	0.00175
***p*TZ2a**	0.00986	0.00152
***p*TZ3a**	0.00979	0.00146
***p*TZ4a**	0.00977	0.00144
***p*TZ5a**	0.01402	0.00201
***p*TZ0b**	0.01259	0.00054
***p*TZ1b**	0.01245	0.0003
***p*TZ2b**	0.01239	0.00024
***p*TZ3b**	0.01236	0.00022
***p*TZ4b**	0.01236	0.00021

Table. S10. Calculated zero-field splitting parameters of the Q state of anthracene-radical linked π-conjugated spin systems by ROBP/ESR-II.

Sample	D_{SS} / cm^{-1}	E_{SS} / cm^{-1}
***p*IN0a**	0.01401	0.00141
***p*IN1a**	0.01222	0.00017
***p*IN2a**	0.01184	0.00012
***p*IN3a**	0.01163	0.00019
***p*IN4a**	0.01150	0.00021
***p*IN5a**	0.01161	0.00027
***p*IN0b**	0.01385	0.00252
***p*IN1b**	0.01070	0.00207
***p*IN2b**	0.00969	0.00192
***p*IN3b**	0.00934	0.00185
***p*IN4b**	0.00921	0.00182
***p*OV0a**	0.01394	0.00151
***p*OV1a**	0.01236	0.00017
***p*OV2a**	0.01186	0.00009
***p*OV3a**	0.01167	0.00018
***p*OV4a**	0.01153	0.00021
***p*OV5a**	0.01161	0.00027
***p*OV0b**	0.01439	0.00279
***p*OV1b**	0.01079	0.00218
***p*OV2b**	0.00970	0.00195
***p*OV3b**	0.00934	0.00186
***p*OV4b**	0.00921	0.00183
***m*NO0a**	0.01539	0.00236
***m*NO1a**	0.01254	0.00021
***m*NO2a**	0.01198	0.00013
***m*NO3a**	0.01171	0.00020
***m*NO4a**	0.01159	0.00023
***m*NO5a**	0.01148	0.00023
***m*NO0b**	0.01532	0.00232

***m*NO1b**	0.01112	0.00195
***m*NO2b**	0.00983	0.00189
***m*NO3b**	0.00939	0.00185
***m*NO4b**	0.00923	0.00183
***p*NN0a**	0.01353	0.00115
***p*NN1a**	0.01214	0.00006
***p*NN2a**	0.01165	0.00011
***p*NN3a**	0.01158	0.00019
***p*NN4a**	0.01153	0.00023
***p*NN5a**	0.01164	0.00028
***p*NN0b**	0.01385	0.00151
***p*NN1b**	0.01063	0.00185
***p*NN2b**	0.00966	0.00186
***p*NN3b**	0.00933	0.00184
***p*NN4b**	0.00921	0.00182
***p*TZ0a**	--	--
***p*TZ1a**	--	--
***p*TZ2a**	--	--
***p*TZ3a**	--	--
***p*TZ4a**	--	--
***p*TZ5a**	--	--
***p*TZ0b**	--	--
***p*TZ1b**	--	--
***p*TZ2b**	--	--
***p*TZ3b**	--	--
***p*TZ4b**	--	--

Table. S11. Calculated zero-field splitting (zfs) parameters of the Q state of anthracene-radical linked π-conjugated spin systems by UCAM-B3LYP/def2-TZVB. The contributions from the spin-orbit (SO) interaction in the zfs parameters were calculated by the PK method.[10] D_{SO} and E_{SO} are corrected using the pre-factors proposed by van Wüllen[11] in the relationship, D_{SO} (van Wüllen) = D_{SO} (PK) × $2S/(2S-1)$.

Sample	D_{SS} / cm^{-1}	E_{SS} / cm^{-1}	D_{SO} / cm^{-1}	E_{SO} / cm^{-1}
***p*IN0a**	0.01307	0.00282	0.00093	0.00005
***p*IN1a**	0.01159	0.00135	0.00037	0.00026
***p*IN2a**	0.01143	0.00113	-0.00048	0.00064
***p*IN3a**	0.01128	0.00111	-0.00038	0.00055
***p*IN4a**	0.01113	0.00113	-0.00032	0.00056
***p*IN5a**	0.01099	0.00116	0.00229	-0.00034
***p*IN0b**	0.01218	0.00273	0.00416	-0.00111
***p*IN1b**	0.00998	0.00168	0.0045	-0.00114
***p*IN2b**	0.00972	0.00144	0.00473	-0.00099
***p*IN3b**	0.00968	0.00132	0.00502	-0.00096
***p*IN4b**	0.00962	0.00072	0.00511	-0.00045
***p*OV0a**	0.01357	0.00269	0.00127	0.00107
***p*OV1a**	0.01210	0.00119	0.00206	0.00082
***p*OV2a**	0.01197	0.00098	0.0003	0.00157
***p*OV3a**	0.01187	0.00095	0.0003	0.00158
***p*OV4a**	0.01177	0.00096	0.00038	0.00157
***p*OV5a**	0.01167	0.00098	0.00052	0.00161
***p*OV0b**	0.01232	0.0029	0.00369	0.0002
***p*OV1b**	0.00997	0.00176	0.0039	0.00023
***p*OV2b**	0.00973	0.00156	0.00423	0.0002
***p*OV3b**	0.00969	0.00152	0.00468	0.00015
***p*OV4b**	0.00967	0.0015	0.00496	0.00009
***m*NO0a**	-0.01327	-0.00544	-0.00356	-0.00006
***m*NO1a**	0.01228	0.00130	0.00219	0.00198
***m*NO2a**	0.01195	0.00101	0.00233	0.00197

***m*NO3a**	0.01182	0.00097	0.00251	0.00195
***m*NO4a**	0.01178	0.00095	0.00179	0.00215
***m*NO5a**	0.01181	0.00093	0.00087	0.00259
***m*NO0b**	0.01370	0.00287	0.00411	0.00092
***m*NO1b**	0.01016	0.00180	0.00441	0.00108
***m*NO2b**	0.00974	0.00157	0.00464	0.00109
***m*NO3b**	0.00966	0.00151	0.00492	0.00100
***m*NO4b**	0.00963	0.00148	0.00512	0.00092
***p*NN0a**	0.01236	0.00278	0.00399	-0.00069
***p*NN1a**	0.01127	0.00141	0.00452	-0.00087
***p*NN2a**	0.01022	0.00152	0.00225	-0.00006
***p*NN3a**	0.00990	0.00157	0.00163	0.00027
***p*NN4a**	0.01095	0.00082	0.00520	-0.00045
***p*NN5a**	0.01164	0.00028	-0.00136	0.00281
***p*NN0b**	0.01206	0.00201	0.00623	-0.00150
***p*NN1b**	0.00991	0.00168	0.00649	-0.00152
***p*NN2b**	0.00974	-0.00150	0.00684	0.00156
***p*NN3b**	0.00968	-0.00120	0.00704	0.00136
***p*NN4b**	0.00969	-0.00147	0.00735	0.00169
***p*TZ0a**	-0.01037	0.00079	-0.09113	-0.01332
***p*TZ1a**	-0.00778	0.00057	-0.08970	-0.01367
***p*TZ2a**	-0.00741	-0.00120	-0.08881	-0.01342
***p*TZ3a**	-0.00734	-0.00229	-0.09078	-0.01251
***p*TZ4a**	-0.00731	0.00125	-0.09052	-0.01479
***p*TZ5a**	-0.00729	0.00119	-0.09174	-0.01365
***p*TZ0b**	-0.01004	-0.00458	-0.08843	-0.01421
***p*TZ1b**	-0.00755	-0.00409	-0.08921	-0.01506
***p*TZ2b**	-0.00717	-0.00408	-0.08974	-0.01518
***p*TZ3b**	-0.00708	-0.00409	-0.09082	-0.01453
***p*TZ4b**	-0.00703	-0.00408	-0.08921	-0.01550

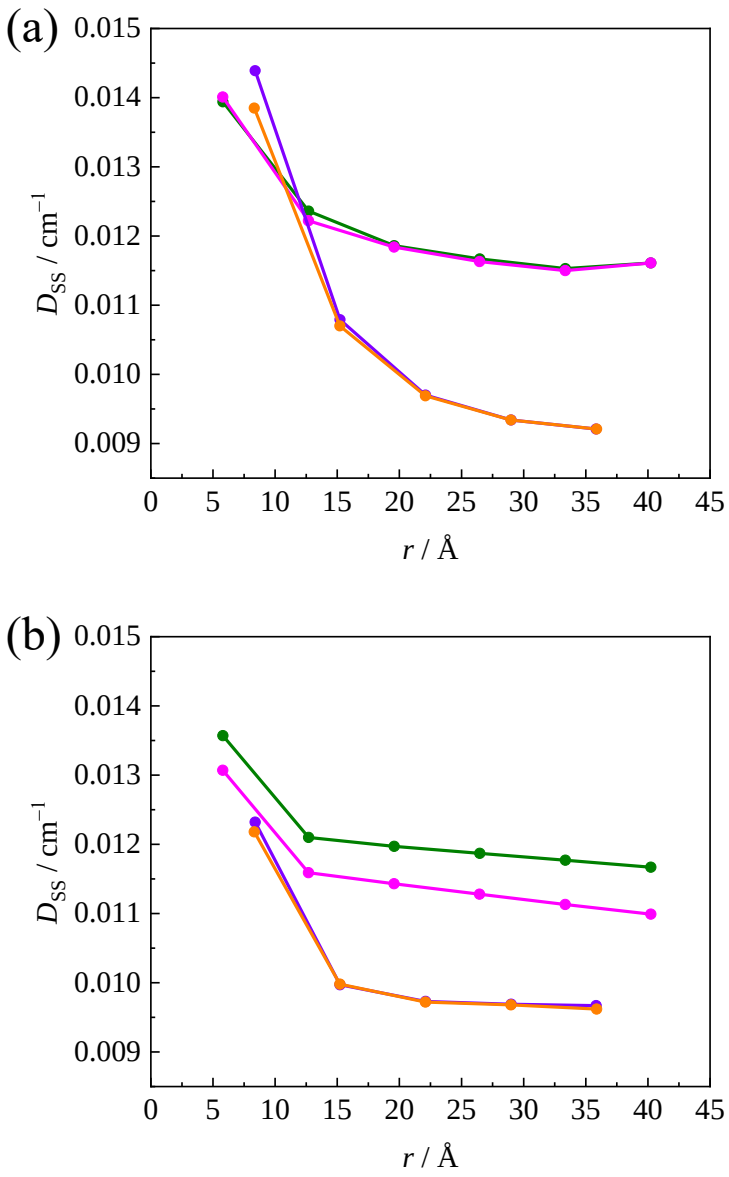

Fig. S7. Calculated *D* values of the Q state of ***p*OVna** (green), ***p*INna** (pink), ***p*OVnb** (violet), and ***p*INnb** (orange) series, by (a) ROBP/ESR-II and (b) UCAM-B3LYP/def2-TZVB.

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